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Minimum Eigenvalue Separation

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Minimum Eigenvalue Separation[1]

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Abstract

Consider real unreduced $n \times n$ symmetric tridiagonal matrices with all sub-diagonal entries equal to one. Such a matrix has distinct real eigenvalues and Parlett conjectured that they must differ by at least

$$2\,(\omega - \frac{1}{\omega})^2/\omega^n = O(\omega^{2-n}),$$

where ω is the spread of diagonal entries and should exceed 4.

We show that the conjecture is true for $\omega > 3n$, but fails if ω/n is too small. The proof rests on two types of lower bound for eigenvalue separations and on detailed estimates of the ratios of entries of eigenvectors; one set for componentwise ratio of two different vectors, another for adjacent entries in the same vector. These results have some independent interest.

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Chapter 1

Preliminaries

1.1 Introduction and Summary

For over one hundred years, the eigenvalue problem has been investigated by mathematicians, physicists, and engineers. Scientists explored the characterization, location, perturbation and computation of eigenvalues, to name a few topics. This thesis is devoted to the separation of eigenvalues. We will find the minimum gap between eigenvalues over an interesting class of tridiagonal matrices.

We consider unreduced $n \times n$ symmetric tridiagonal matrices with all subdiagonal entries 1. The typical matrix may be written

$$J_n(\mathbf{a}) = \text{tridiag}\begin{pmatrix} & 1 & & 1 & \cdots & 1 & \\ a(1) & & a(2) & \cdot & \cdots & \cdot & a(n) \\ & 1 & & 1 & \cdots & 1 & \end{pmatrix}, \qquad (1.1)$$

where $\mathbf{a} = (a(1), a(2), \ldots, a(n))$ denotes the diagonal and $a(k) \in \mathbf{R}$.

$J(\mathbf{a})$ has distinct real eigenvalues and, in [10], Parlett conjectured that they must differ by at least

$$2\,(\omega - \frac{1}{\omega})^2/\omega^n = O(\omega^{2-n}),$$

where $\omega = \max_{1\le k\le n} a(k) - \min_{1\le k\le n} a(k)$ is the spread of diagonal entries and should exceed 4. Our contribution is to settle this conjecture. It is true for $\omega > 3n$ and probably for some smaller ratio ω/n. Nevertheless some condition on ω/n is necessary because we have counter examples for $\omega > 4$.

As will be shown later, the problem of finding the minimal separation of eigenvalues for given n and diagonal spread ω is a piecewise smooth constrained optimization problem.

The first task is to find matrices that satisfy the Kuhn-Tucker conditions, but it is much harder to deduce when these matrices are global extrema. Indeed, when ω is not large enough the rival configurations also satisfy the Kuhn-Tucker conditions and appropriate the global minimum to themselves.

It is not immediately apparent but the eigenvalue gap does not start to get small until a few eigenvalues are clearly separated from the others. This observation directs our attention to the case $\omega > 4$.

The proof rests on detailed estimates of the ratios of entries of eigenvectors; one set for componentwise ratio of two different vectors, another for adjacent entries in the same vector. These results have some independent interest.

The motivation leads us to the definition of minimum eigenvalue separation, or gap.

Definition 1 *Let $\{\lambda_i\}$ be the set of eigenvalues of a matrix A, then the gap of A's spectrum is*

$$g(A) := \min_{i \neq j} |\lambda_i - \lambda_j|.$$

In section 1.2 we survey some of the voluminous literature on gap. We also include results on the first excitation energy of the Schrödinger operator. We show, in section 1.3, that the minimal gap is invariant under shift, duality, reversal of the diagonal, and their combinations. In section 1.4 we normalize and formulate our minimization problem, and give a complete description of the answer. When ω is large enough, $\mathbf{w_1} = (\omega, 0, \ldots, 0, \omega)$ becomes the minimizer. We compute the gradient of each eigenvalue separation with respect to the diagonal in section 1.5. Section 1.6 includes formulas for the entries of normalized eigenvectors and their symmetric properties.

Chapter 2 is devoted to our extremal matrix $J(\mathbf{w_1})$. Its eigenvalue equation and eigenvectors can be expressed in terms of Chebyshev polynomials. By symbolic computation, we can derive the asymptotic expansions of two dominant eigenvalues and hence their separation. Precise bounds are included as well. We also have the analogue for the dual matrix $J(\mathbf{w_1^*})$.

Chapter 3 explores the ratios of the entries of eigenvectors. Let λ_n and λ_{n-1} be two largest eigenvalues with corresponding eigenvectors $\mathbf{v_n}$ and $\mathbf{v_{n-1}}$. We prove that the ratio $\frac{v_{n-1}(k)}{v_n(k)}$ is strictly monotonic as k increases. It follows that $\nabla(\lambda_n - \lambda_{n-1})$ obeys certain

sign pattern. Ashbaugh and Benguria's Comparison Theorem [1] is an easy consequence. We also have inequalities for the ratios $\frac{v_n(k+1)}{v_n(k)}$ and $\frac{v_{n-1}(k+1)}{v_{n-1}(k)}$, and establish convexity for the components of an eigenvector.

Chapter 4 solves our minimization problem when the size of diagonal spread is large enough. Suppose the eigenvalues are in increasing order $\lambda_1 < \lambda_2 < \cdots < \lambda_n$. We obtain a lower bound for each $\lambda_{i+1} - \lambda_i$, which indicates the middle ones always have bigger lower bounds than $\lambda_2 - \lambda_1$ and $\lambda_n - \lambda_{n-1}$. Hence the middle separations can not compete with the end ones. By duality we only need to consider $\lambda_n - \lambda_{n-1}$. From the refinement of Sun's theorem, the trace of the minimal matrix must be small. In view of the Kuhn-Tucker condition, the sign patterns of $\nabla(\lambda_n - \lambda_{n-1})$ yield all the possible local minimizers. Then we use the ratio inequalities from the previous chapter to eliminate the unsymmetric minimizers. Finally we prove $J(\mathbf{w_1})$ indeed minimizes $\lambda_n - \lambda_{n-1}$ locally. We sketch the whole process and state the main theorem in section 4.5.

1.2 Review of the Literature

The gap of a matrix indicates whether its spectrum is well separated. Hence the separation of eigenvalues is closely related to the difficulty of eigenvalue computation. In fact the number of iterations of many methods depends on the size of the gap.

Wilkinson [15, p. 308] studied

$$W_{2m+1} = J_{2m+1}(\mathbf{a}) \qquad \text{with} \quad a(k) = |m+1-k| \quad \text{for } k = 1, 2, \ldots, 2m+1.$$

The largest two eigenvalues of W_{2m+1} differ by roughly $(m!)^{-2}$. For example λ_{20} and λ_{21} of W_{21} agree for their first fifteen decimal digits! Nevertheless this is not the smallest gap for such matrices.

Wang [14] generalizes Wilkinson's matrix W_{2m+1} to

$$W_{2m+1}(d) = J_{2m+1}(\mathbf{a}') \qquad \text{with} \quad a'(k) = |m+1-k|\, d \quad \text{for } k = 1, 2, \ldots, 2m+1.$$

Then he gives upper and lower bounds for its gap.

Theorem 1.1 (Wang) *For* $d \geq 0.92$,

$$\frac{1}{2m(m!)^2 d^{2m-1}} < g(W_{2m+1}(d)) < \frac{30m^2}{(m!)^2 d^{2m-1}}.$$

Sun [12, Theorem 1] considers real tridiagonal matrix

$$T_n = \text{tridiag}\begin{pmatrix} & b_1 & & b_2 & \cdots & b_{n-1} & \\ a_1 & & a_2 & \cdot & \cdots & \cdot & a_n \\ & c_2 & & c_3 & \cdots & c_n & \end{pmatrix} \text{ with } b_{k-1}c_k > 0 \text{ for } k = 2, 3, \cdots, n, \tag{1.2}$$

and gives a lower bound for gap.

Theorem 1.2 (Sun) *For $n > 2$,* $\quad g(T_n) > 2\,(\prod_{k=2}^{n} b_{k-1}c_k)^{\frac{1}{2}}\, p^{2-n}$ $\quad$ *where*

$$p = min\{p_1, max(p_2, p_3)\}, \qquad p_1 = \overline{\lambda}_n - \underline{\lambda}_1,$$

$$p_2 = \frac{1}{n-2}(n\overline{\lambda}_n - \sum_{k=1}^{n} a_k), \qquad p_3 = \frac{1}{n-2}(\sum_{k=1}^{n} a_k - n\underline{\lambda}_1),$$

$$\overline{\lambda}_n = \max_{1\le k\le n}\{a_k + |b_k| + |c_k|\}, \qquad \underline{\lambda}_1 = \min_{1\le k\le n}\{a_k - |b_k| - |c_k|\},$$

$$\textit{and} \qquad c_1 = b_n = 0.$$

We mention that $\underline{\lambda}_1$ and $\overline{\lambda}_n$ given in his paper are misprints. $\underline{\lambda}_1$ should be a lower bound for the smallest eigenvalues of T_n and $\overline{\lambda}_n$ an upper bound for the largest one. They can be estimated by the Gershgorin's Disk Theorem. For example W_{2m+1} has

$$\overline{\lambda}_n = m + 1 \qquad \text{and} \qquad \underline{\lambda}_1 = -2.$$

While the deleted absolute row sums are used in Theorem 1.2, we may have following different choices by columns

$$\overline{\lambda}_n = \max_{1\le k\le n}\{a_k + |b_{k-1}| + |c_{k+1}|\}, \quad \underline{\lambda}_1 = \min_{1\le k\le n}\{a_k - |b_{k-1}| - |c_{k+1}|\},$$

with $b_0 = c_{n+1} = 0$.

Note that Theorem 1.2 can be improved and the refinement is stated in Theorem 4.3. Table 1.1 compares the true value and several lower bounds from Theorem 1.1-3 and 4.3 for the gap of W_{21}. In fact Sun uses

$$\lambda_n(W_{2m+1}) - \lambda_{n-1}(W_{2m+1}) > 2p_2^{2-n} = 2\,(\frac{2m-1}{m^2+2m+1})^{2m-1}$$

instead of Theorem 1.2 to get the bound 1.06×10^{-15} in the table.

Sun's [12, Theorem 2] for gap is wrongly stated since he mistakes $|2\chi'(\lambda_i)/\chi''(\lambda_i)|$ for $|\lambda_{i+1} - \lambda_i|$, where $\chi(\lambda) = det(\lambda I - T)$ and eigenvalues $\{\lambda_i\}$ of T are in increasing order. The true formula is

$$\frac{\chi''(\lambda_i)}{2\chi'(\lambda_i)} = \sum_{\substack{k=1\\k\ne i}}^{n} \frac{1}{\lambda_i - \lambda_k}.$$

true gap	Theorem 1.1	Theorem 1.2	Theorem 1.3	Theorem 4.3
7×10^{-14}	3.8×10^{-15}	1.06×10^{-15}	1.07×10^{-15}	1.24×10^{-15}

Table 1.1: Low bounds for $g(W_{21})$.

The minimum eigenvalue separation of two matrices is defined as following. Let $\{\lambda_i\}$ and $\{\mu_j\}$ be eigenvalues of matrices A and B respectively, where A and B may have different dimensions. Then for all pairs of λ_i and μ_j,

$$g(A,B) := \min_{i,j} |\lambda_i - \mu_j|.$$

Recall $\underline{\lambda}_1$ and $\overline{\lambda}_n$ given in Theorem 1.2.

Theorem 1.3 (Sun [12]) *The tridiagonal matrices T_n and T_{n-1} given by (1.2) have separation*

$$g(T_{n-1}, T_n) > \prod_{k=2}^{n} b_{k-1}c_k \cdot \max\{\tilde{p}^{3-2n},\ p(n)^{1-n}p(n-1)^{2-n}\},$$

where $\tilde{p}_1 = \overline{\lambda}_n - \underline{\lambda}_1$, $\tilde{p}_2 = \frac{1}{2n-3}[(2n-1)\overline{\lambda}_n - tr(T_n) - tr(T_{n-1})]$,
$\tilde{p}_3 = \frac{1}{2n-3}[tr(T_n) + tr(T_{n-1}) - (2n-1)\underline{\lambda}_1]$, $\tilde{p} = \min\{\tilde{p}_1,\ \max(\tilde{p}_2,\ \tilde{p}_3)\}$,
$p(j) = \min\{\tilde{p}_1,\ \max(p_2(j), p_3(j))\}$, $p_2(j) = \frac{1}{j-1}[j\overline{\lambda}_n - tr(T_j)]$,
$p_3(j) = \frac{1}{j-1}[tr(T_j) - j\underline{\lambda}_1]$, *for* $j = n,\ n-1$.

We remark that a centrosymmetric matrix, which is symmetric with respect to both long diagonals, can be split into two smaller matrices such that each one owns half of the original spectrum [3]. See section 1.6 for more detail. Therefore $g(W_{21})$ is equal to the gap between two submatrices, and we can estimate $g(W_{21})$ by Theorem 1.3. The lower bound is listed on Table 1.1.

In quantum mechanics, an eigenvalue corresponds to the energy level of a certain state. A separation of eigenvalues thus represents the energy absorbed (or emitted) in the transition from one state to another. A lot of recent research by physicists has focussed on the first excitation energy, or in mathematical terms, the separation between the first two eigenvalues. We give a brief survey of that literature here.

First cousider the Schrödinger operator in general dimension n. It is well known that the lowest eigenvalue of the Schrödinger operator is always non-degenerate. Hence it makes sense to discuss the gap between the first and the second eigenvalues.

Let Ω be a smooth strictly convex bounded domain in $\mathbf{R}^n$, potential $V : \Omega \to \mathbf{R}$ be a nonnegative convex function, and Δ be the Laplace operator. The eigenvalues of

$$\begin{cases} -\Delta f + V(x) f = \lambda f, \\ f = 0 \quad \text{on } \partial\Omega, \end{cases}$$

can be arranged in nondecreasing order $0 < \lambda_1 \leq \lambda_2 \leq \lambda_3 \leq \cdots$. Singer, Wang, Yau, and Yau [11] prove that

$$\lambda_2 - \lambda_1 \geq \frac{\pi^2}{4d^2},$$

where d is the diameter of Ω. Under the same hypotheses, Yu and Zhong [16] improve the estimate to

$$\lambda_2 - \lambda_1 \geq \frac{\pi^2}{d^2}.$$

Kirsch and Simon [7] give a Comparison Theorem for $\lambda_2 - \lambda_1$ of two different Schrödinger operators and use it to find new bounds on the lowest band in a solid. For bounded potential $V(x)$, they also give a lower bound for $\lambda_2 - \lambda_1$ depending on the geometry of the set $C = \{x | V(x) < \lambda_2\}$ and the maximum value of $|V(x) - \nu|$ over the convex hull of C and $\nu \in [\lambda_1, \lambda_2]$.

For the one dimensional case, the Schrödinger operator becomes $-\frac{d^2}{dx^2} + V(x)$ in an interval. It is also known that all the eigenvalues are nondegenerate and can be ordered by $\lambda_1 < \lambda_2 < \lambda_3 < \cdots$. Hence each separation $\lambda_{i+1} - \lambda_i$ never vanishs.

Kirsch and Simon [6] provide the same type of lower bounds for $\lambda_{i+1} - \lambda_i$ in one dimension as in [7]. Consider $-\frac{d^2}{dx^2} + V(x)$ on $[a, b]$ with either Dirichlet or Neumann boundary conditions at a and b. Assume $V \in C^\infty([a, b])$ and

$$\gamma_i = \max\{\, |\nu - V(x)|^{\frac{1}{2}} : x \in (a, b) \text{ and } \nu \in (\lambda_i, \lambda_{i+1})\},$$

then

$$\lambda_{i+1} - \lambda_i \geq \pi \gamma_i^2 \exp[-\gamma_i (b - a)].$$

The exponential factor in such bounds are realized precisely in tunneling examples.

For the one dimensional Schrödinger operator with a symmetric single well potential $V(x)$ in a interval of length d and with Dirichlet boundary conditions, Ashbaugh and

Benguria [2] obtain the optimal lower bound

$$\lambda_2 - \lambda_1 \geq \frac{3\pi^2}{d^2}.$$

Equality holds if and only if the potential is constant. A single well potential in $[a, b]$ means there is a $c \in [a, b]$ such that V is nonincreasing for $x \leq c$ and nondecreasing for $x \geq c$.

The lower bound for $\lambda_2 - \lambda_1$ comes from a general comparison theorem which is stated below. Consider two Schrödinger operators $-\frac{d^2}{dx^2} + U(x)$ and $-\frac{d^2}{dx^2} + V(x)$ with Dirichlet boundary conditions. Let $\{\lambda_i(U)\}$ and $\{\lambda_i(V)\}$ be their eigenvalues respectively. Assume both U and V are centrally symmetric, and $U - V$ is a single well potential, then

$$\lambda_2(U) - \lambda_1(U) \geq \lambda_2(V) - \lambda_1(V)$$

and the equality holds if and only if $U - V$ is constant.

The discrete analogue of Schrödinger operator is a tridiagonal matrix of the form $-L + D$, where L is the discrete laplacian

$$L = \text{tridiag}\begin{pmatrix} & 1 & & 1 & \cdots & 1 & \\ -2 & & -2 & \cdot & \cdots & \cdot & -2 \\ & 1 & & 1 & \cdots & 1 & \end{pmatrix}$$

and D is a diagonal matrix. Thus all the previous problems reduce to estimating the gap between two adjacent eigenvalues of tridiagonal matrices.

Ashbaugh and Benguria published the discrete version of their results in [1]. For example their Comparison Theorem becomes

$$\lambda_2(-L + \tilde{D}) - \lambda_1(-L + \tilde{D}) \geq \lambda_2(-L + D) - \lambda_1(-L + D),$$

if the diagonals of $\tilde{D}$ and D are centrally symmetric, and that of $\tilde{D} - D$ is symmetric increasing from the midpoint. In Chapter 3, we will provide a simple proof of this Comparison Theorem using our eigenvectors' ratios.

1.3 Symmetries

Only symmetric tridiagonal matrices are considered in this paper. The eigenvalue problem is trivial for diagonal and bidiagonal matrices. So the simplest nontrivial form is the tridiagonal. However there is no loss of generality since every symmetric matrix is orthogonally equivalent to a symmetric tridiagonal matrix. In fact we assume all subdiagonal

entries nonzero. Such tridiagonal matrices are called *unreduced*. In case some subdiagonal entries vanish, then the matrix becomes block diagonal with each block an unreduced tridiagonal. We can take care of eigenvalues of each unreduced submatrices separately.

The unreduced symmetric tridiagonal matrices have the form

$$T(\mathbf{a}) = \mathrm{tridiag}\begin{pmatrix} & \beta_1 & & \beta_2 & \cdots & \beta_{n-1} & \\ a(1) & & a(2) & \cdot & \cdots & \cdot & a(n) \\ & \beta_1 & & \beta_2 & \cdots & \beta_{n-1} & \end{pmatrix},$$

where $\mathbf{a} = (a(1), a(2), \ldots, a(n))$ is the diagonal, and all the β_i's are nonzero. The tridiagonal matrix T_n in (1.2) can be symmetrized to the form $T(\mathbf{a})$ by scaling. More precisely, there is a diagonal matrix D such that

$$T(\mathbf{a}) = D\,T_n\,D^{-1},$$

where $a(k) = a_k$ for $k = 1, 2, \ldots, n$, and $\beta_k = \pm\sqrt{b_k c_{k+1}}$ for k=1, 2, …, $n-1$.

Before formulating our minimization problem, it is necessary to understand the behavior of eigenvalue separations. In this section we will accumulate the background needed. We start with some invariant properties of eigenvalues and eigenvectors, and then explore symmetries under which gap is invariant.

Let $\{\lambda_i(\mathrm{T})\}$ and $\{\mathbf{s_i}(T)\}$ be the eigenvalues and corresponding normalized eigenvectors of matrix T. It's well known that an unreduced symmetric tridiagonal matrix has distinct real eigenvalues [9, 7-7-1]. In this paper we always order λ_i increasingly, i.e.

$$\lambda_1 < \lambda_2 < \cdots < \lambda_n.$$

Define the i-th eigenvalue separation to be

$$g_i(T) := \Delta\lambda_i(T) = \lambda_{i+1}(T) - \lambda_i(T),$$

where Δ is the forward difference. Then the gap defined by Definition 1 is equivalent to

$$g(T) = \min_{1\le i\le n-1} g_i(T). \tag{1.3}$$

For every eigenvector $\mathbf{s_i}$, the first entry $s_i(1)$ and the last one $s_i(n)$ are always nonzero [9, 7-9-5]. An easy way to see this is from the three-term recurrence; $\mathbf{s_i} = 0$ if $s_i(1) = 0$. Hence without loss of generality, we can assume $s_i(1) > 0$ for all i's.

Theorem 1.4 *Let* $\hat{I} = \begin{pmatrix} 1 & & & & \\ & -1 & & & \\ & & 1 & & \\ & & & -1 & \\ & & & & \ddots \end{pmatrix}$, $\tilde{I} = \begin{pmatrix} & & & & 1 \\ & & & 1 & \\ & & ⋰ & & \\ & 1 & & & \\ 1 & & & & \end{pmatrix}$, $\mathbf{e} = \begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \\ 1 \end{pmatrix}$,

$\mathbf{a} = (a(1), a(2), \ldots, a(n))^T$ *and* σ *be a scalar, then for* $i = 1, 2, \ldots, n$,

i. $\lambda_i(T(\mathbf{a} + \sigma\mathbf{e})) = \lambda_i(T(\mathbf{a})) + \sigma$, *and* $\mathbf{s_i}(T(\mathbf{a} + \sigma\mathbf{e})) = \mathbf{s_i}(T(\mathbf{a}))$,

ii. $\lambda_i(T(-\mathbf{a})) = -\lambda_{n-i}(T(\mathbf{a}))$, *and* $\mathbf{s_i}(T(-\mathbf{a})) = \hat{I}\,\mathbf{s_i}(T(\mathbf{a}))$,

iii. $\lambda_i(T(\sigma\mathbf{e} - \mathbf{a})) = \sigma - \lambda_{n-i}(T(\mathbf{a}))$, *and* $\mathbf{s_i}(T(\sigma\mathbf{e} - \mathbf{a})) = \hat{I}\,\mathbf{s_i}(T(\mathbf{a}))$,

iv. assume in addition $\beta_j = \beta_{n-j}$ *for* $j = 1, 2, \ldots, n-1$, *then*

$\lambda_i(T(\tilde{I}\mathbf{a})) = \lambda_i(T(\mathbf{a}))$, *and* $\mathbf{s_i}(T(\tilde{I}\mathbf{a})) = \tilde{I}\,\mathbf{s_i}(T(\mathbf{a}))$.

Proof.

i. Since $T(\mathbf{a} + \sigma\mathbf{e}) = T(\mathbf{a}) + \sigma I$,

$$\lambda_i(T(\mathbf{a} + \sigma\mathbf{e})) = \lambda_i(T(\mathbf{a})) + \sigma$$

and eigenvector $\mathbf{s_i}(T(\mathbf{a} + \sigma\mathbf{e}))$ remains unchanged.

ii. Observe that $\hat{I}^{-1} = \hat{I}$ and $\hat{I}T(\mathbf{a})\hat{I} = -T(-\mathbf{a})$. Since eigenvalues are ordered increasingly, $\lambda_i(T(-\mathbf{a})) = \lambda_i(-\hat{I}T(\mathbf{a})\hat{I}) = \lambda_i(-T(\mathbf{a})) = -\lambda_{n-i}(T(\mathbf{a}))$. Also

$$\mathbf{s_i}(T(-\mathbf{a})) = \mathbf{s_i}(-T(-\mathbf{a})) = \mathbf{s_i}(\hat{I}T(\mathbf{a})\hat{I}) = \hat{I}\,\mathbf{s_i}(T(\mathbf{a})).$$

iii. Combine previous two,

$$\lambda_i(T(\sigma\mathbf{e} - \mathbf{a})) = \sigma + \lambda_i(T(-\mathbf{a})) = \sigma - \lambda_{n-i}(T(\mathbf{a}))$$

and

$$\mathbf{s_i}(T(\sigma\mathbf{e} - \mathbf{a})) = \mathbf{s_i}(T(-\mathbf{a})) = \hat{I}\,\mathbf{s_i}(T(\mathbf{a})).$$

iv. By the symmetry of β_j's, $\tilde{I}T(\mathbf{a})\tilde{I} = -T(\tilde{I}\mathbf{a})$. Since $\tilde{I}^{-1} = \tilde{I}$,

$$\lambda_i(T(\tilde{I}\mathbf{a})) = \lambda_i(T(\mathbf{a})) \quad \text{and} \quad \mathbf{s_i}(T(\tilde{I}\mathbf{a})) = \mathbf{s_i}(\tilde{I}T(\mathbf{a})\tilde{I}) = \tilde{I}\,\mathbf{s_i}(T(\mathbf{a})).$$

□

Although eigenvalues are invariant under all similarity transforms, not many of them preserve the tridiagonal structure. $\hat{I}$ and $\bar{I}$ are among such few examples. Notice that vector $\bar{I}\mathbf{a}$ is just the reverse order of $\mathbf{a}$.

Definition 2 *Given vector* $\mathbf{a} = (a(1), a(2), \ldots, a(n))$ *and scalar* ω.

i. We denote the reverse order of $\mathbf{a}$

$$\mathbf{a}^R := \bar{I}\mathbf{a} = (a(n), a(n-1), \ldots, a(1)).$$

ii. We define the dual of $\mathbf{a}$ *with respect to* ω *by*

$$\mathbf{a}^* := \omega\mathbf{e} - \mathbf{a} = (\omega - a(1), \omega - a(2), \ldots, \omega - a(n)).$$

The duality is the combination of shift and reflection about origin. Of course we can combine different operations in Theorem 1.4 to get other symmetries.

As a simple consequence of Theorem 1.4, the gap is invariant under shift, reflection with respect to origin, and duality. In addition if β_j's are symmetric, then it's invariant under reversing diagonal.

Corollary 1.5 *Assume* $\mathbf{e}, \mathbf{a}, \sigma$ *are the same as in Theorem 1.4, then for* $i = 1, 2, \ldots, n$

i. $g_i(T(\mathbf{a} + \sigma\mathbf{e})) = g_i(T(\mathbf{a}))$, *and* $g(T(\mathbf{a} + \sigma\mathbf{e})) = g(T(\mathbf{a}))$,

ii. $g_i(T(-\mathbf{a})) = g_{n-i}(T(\mathbf{a}))$, *and* $g(T(-\mathbf{a})) = g(T(\mathbf{a}))$,

iii. $g_i(T(\mathbf{a}^*)) = g_{n-i}(T(\mathbf{a}))$, *and* $g(T(\mathbf{a}^*)) = g(T(\mathbf{a}))$,

iv. assume in addition $\beta_j = \beta_{n-j}$ *for* $j = 1, 2, \ldots, n-1$, *then*

$g_i(T(\mathbf{a}^R)) = g_i(T(\mathbf{a}))$, *and* $g(T(\mathbf{a}^R)) = g(T(\mathbf{a}))$

1.4 Normalization of the Problem

One certainly can try to find a tridiagonal matrix with gap smaller than that of W_{2n+1}, but we ask a more general question: what is the minimal gap over this type of matrix? To make this minimization problem well posed, some normalization is needed. A few simple observations will help:

unreduced tridiagonal Our problem becomes trivial unless we exclude those matrices with multiple eigenvalues, e.g. the identity matrix. Therefore we only consider unreduced tridiagonal matrices which always have distinct eigenvalues.

symmetric tridiagonal Also we only deal with symmetric case so that all the eigenvalues are real. The gap certainly can be defined, in a similar fashion, for complex eigenvalues. But it is more difficult to analyze.

β_k's bounded below The off-diagonal elements play an important role for the distribution of eigenvalues. Consider

$$\begin{pmatrix} 0 & \epsilon \\ \epsilon & 0 \end{pmatrix}$$

whose eigenvalues are $\pm\epsilon$. Its gap 2ϵ has no lower bound if we let $\epsilon \to 0$. Therefore we need to fix a lower bound on the off-diagonal elements.

scalar multiplication Notice that the gap function is homogeneous under scalar multiplication, i.e.

$$g(\sigma T) = \sigma\, g(T)$$

for all scalar σ. Hence we can fix all the off-diagonal elements $\beta_k \geq 1$, which is just a normalization constant.

n=2 The eigenvalues of $J_2(a)$ are

$$\frac{1}{2}[a(1) + a(2) \pm \sqrt{(a(1) - a(2))^2 + 4}\,].$$

Hence the gap

$$\sqrt{(a(1) - a(2))^2 + 4} \geq 2.$$

Equality holds if and only if $a(1) = a(2)$. Therefore there are infinitely many minimizers. From now on only $n > 2$ is considered.

diagonal spread The size of the diagonal spread is crucial. In the next chapter we will show that $J(\mathbf{w_1})$ has gap approximately $2/\omega^{n-2}$, which can be as small as possible when ω is not bounded. Hence the diagonal spread has to be fixed.

shift By the shift invariance Corollary 1.5(i), we can take $\min_{1\leq k\leq n} a(k) = 0$. Assume the diagonal spread is ω, then $\max_{1\leq k\leq n} a(k) = \omega$. In other words we restrict all the diagonal $a(i)$'s to lie in the interval $[0, \omega]$ and in no smaller interval.

ω	[0, 0.1]	[0.2, 0.5]	[0.6, 1.5]	[1.6, 4]	[4.1, ∞]
$\mathbf{a}$	$\mathbf{w_5}$	$\mathbf{w_4}$	$\mathbf{w_3}$	$\mathbf{w_2}$	$\mathbf{w_1}$

Table 1.2: Minimizers for $g(J(\mathbf{a}))$ with $n = 15$.

n fixed The dimension n of the matrix can not be free either. The eigenvalues of $\frac{1}{2}J_n(0)$ are the roots of the n-th order Chebyshev polynomial of second kind, i.e. $cos\frac{k\pi}{n+1}$ for k=1,2,...,n. Hence

$$g(J_n(0)) = 2\cos\frac{\pi}{n+1} - 2\cos\frac{2\pi}{n+1} = 4\sin\frac{3\pi}{2(n+1)}\sin\frac{\pi}{2(n+1)} \approx \frac{3\pi^2}{(n+1)^2}$$

when n is large.

Now we can formulate a well defined minimization problem. For $n \geq 3$ and $\omega > 0$ given, we seek

$$\min g(J(\mathbf{a})) \qquad \text{subject to} \quad 0 \leq a(i) \leq \omega \quad \text{for } i = 1, 2, \ldots, n. \tag{1.4}$$

Parlett [10] conjectures that $J(\mathbf{w_1})$ minimizes (1.4) for $\omega \geq 4$. But in fact the minimizing matrix depends on the size of the diagonal spread ω. Let

$$\mathbf{w_j}(\omega) := (\underbrace{\omega, \ldots, \omega}_{j}, 0, \ldots, 0, \underbrace{\omega, \ldots, \omega}_{j})$$

for $j = 1, 2, \ldots, [\frac{n}{2}]$. Table 1.2 shows the extremal $\mathbf{w_j}(\omega)$ for different size of ω when $n = 15$. $\mathbf{w_5}$ has smallest gap initially, and $\mathbf{w_4}$ beats $\mathbf{w_5}$ after a while, then $\mathbf{w_3}$ takes over and loses to $\mathbf{w_2}$ later. In the end $\mathbf{w_1}$ wins the crown when ω is large enough.

For the general n, $\mathbf{w}_{[\frac{n}{3}]}$ is the starting minimizer for tiny ω, and then $\mathbf{w}_{[\frac{n}{3}]-1}, \ldots,$ etc. For large ω, $\mathbf{w_1}$ is the ultimate winner, and this will be proved in Chapter 4. Therefore (1.4) is not a simple algebraic problem.

Corollary 1.5(iii) shows that $J(\mathbf{w_j})$ and $J(\mathbf{w_j}^*)$ have the same gap, where

$$\mathbf{w_j}^* := (\underbrace{0, \ldots, 0}_{j}, \omega, \ldots, \omega, \underbrace{0, \ldots, 0}_{j})$$

is the dual of $\mathbf{w_j}$. Hence $\mathbf{w_j}^*$ is also a minimizer if $\mathbf{w_j}$ is. Thus (1.4) has at least two minimizers.

Our final remark is that $J_{2m+1}(\mathbf{w_1}(m))$ has smaller gap than W_{2m+1}. Indeed

$$g(J_{2m+1}(\mathbf{w_1}(m))) \approx \frac{2}{m^{2m-1}} \qquad \text{and} \qquad g(W_{2m+1}) \approx (m!)^{-2}.$$

For example, $g(J_{21}(\mathbf{w_1}(10))) = 2 \times 10^{-19}$ while $g(W_{21}) = 7 \times 10^{-14}$.

1.5 Gradient of g_i

In this section we fix all the subdiagonal entries β_k's, and consider λ_i and g_i as a function of the diagonal $\mathbf{a}$. It is surprising that $\nabla g_i = \nabla_{\mathbf{a}} g_i$ has a simple form. Recall that $\mathbf{s_i}$ is the normalized eigenvector of λ_i, i.e.

$$T(\mathbf{a})\mathbf{s_i} = \lambda_i \mathbf{s_i} \tag{1.5}$$

and

$$||\mathbf{s_i}||_2^2 = \mathbf{s_i}^T \mathbf{s_i} = 1 \tag{1.6}$$

Definition 3 *The Schur product of vectors* $\mathbf{u}$ *and* $\mathbf{v}$ *is an element-by-element multiplication*

$$\mathbf{u} \circ \mathbf{v} := (u(1)v(1), u(2)v(2), \ldots, u(n)v(n)).$$

For example consider $\hat{\mathbf{e}} = (1, -1, 1, -1, \ldots)$, then in Section 1.3 $\hat{I}\mathbf{v} = \hat{\mathbf{e}} \circ \mathbf{v}$.

Lemma 1.6 *i.* $\nabla \lambda_i(T(\mathbf{a})) = \mathbf{s_i} \circ \mathbf{s_i}$ *for* $i = 1, 2, \ldots, n$,

ii. $\nabla g_i(T(\mathbf{a})) = \mathbf{s_{i+1}} \circ \mathbf{s_{i+1}} - \mathbf{s_i} \circ \mathbf{s_i}$ *for* $i = 1, 2, \ldots, n-1$.

Proof. Take partial derivatives of (1.5) with respect to a(j)

$$[\frac{\partial}{\partial a(j)} T(\mathbf{a})]\mathbf{s_i} + T(\mathbf{a})\frac{\partial}{\partial a(j)}\mathbf{s_i} = \frac{\partial \lambda_i}{\partial a(j)}\mathbf{s_i} + \lambda_i \frac{\partial}{\partial a(j)}\mathbf{s_i}.$$

Premultiply by $\mathbf{s_i}$ and use (1.6), then

$$\mathbf{s_i}^T diag(\ldots, 0, \underbrace{1}_{\text{j-th}}, 0, \ldots)\,\mathbf{s_i} + \mathbf{s_i}^T T(\mathbf{a})\frac{\partial}{\partial a(j)}\mathbf{s_i} = \frac{\partial \lambda_i}{\partial a(j)}\mathbf{s_i}^T\mathbf{s_i} + \lambda_i \mathbf{s_i}^T \frac{\partial}{\partial a(j)}\mathbf{s_i},$$

$$\mathbf{s_i}(j)^2 + [\lambda_i \mathbf{s_i}]^T \frac{\partial}{\partial a(j)}\mathbf{s_i} = \frac{\partial \lambda_i}{\partial a(j)} + \lambda_i \mathbf{s_i}^T \frac{\partial}{\partial a(j)}\mathbf{s_i},$$

$$\frac{\partial \lambda_i}{\partial a(j)} = s_i(j)^2 \qquad \text{for } i, j = 1, 2, \ldots, n.$$

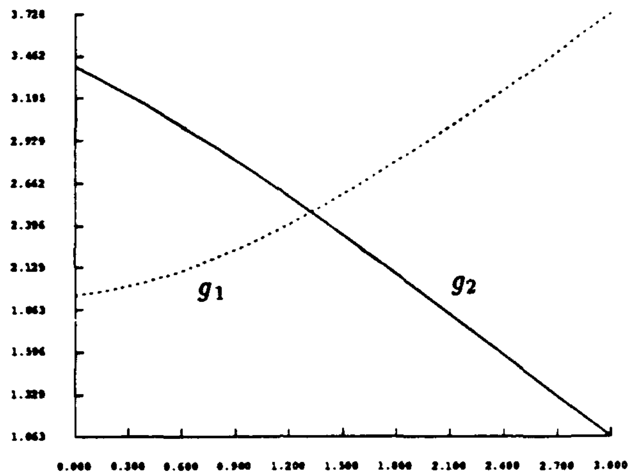

Figure 1.1: g_1 and g_2 for $J_3((4,0,x))$.

Thus for $i = 1, 2, \ldots, n$

$$\nabla\lambda_i = \mathbf{s_i} \circ \mathbf{s_i} \qquad \text{and} \qquad \nabla g_i = \nabla\lambda_{i+1} - \nabla\lambda_i = \mathbf{s_{i+1}} \circ \mathbf{s_{i+1}} - \mathbf{s_i} \circ \mathbf{s_i}.$$

□

By Definition 1 of gap, or by (1.3), we expect that $g(T(\mathbf{a}))$ fails to be differentiable at certain values of $\mathbf{a}$. But restricted to each open domain where $g = g_i$ for some i, ∇g is just ∇g_i. For example, in Figure 1.1 we plot g_1 and g_2 for $J_3((4,0,x))$ with respect to x in $[0,3]$. It is clear that $g = g_1$ when $x \leq 1.3$, and $g = g_2$ when $x \geq 1.3$. Indeed g is not differentiable at the intersection $x = 1.3$.

Before we carry on, we need to clear up our notation. Consider a smooth function $h : \mathbf{R}^n \to \mathbf{R}^n$, $\nabla_a\, g_i(T(h(\mathbf{a})))$ represents the gradient of the composite function of $T(h(\mathbf{a}))$ and g_i with respect to $\mathbf{a}$, while $\nabla g_i(T(h(\mathbf{a})))$ means the evaluation of ∇g_i at $T(h(\mathbf{a}))$. Note that

$$\nabla_a\, g_i(T(\mathbf{a})) = \nabla g_i(T(\mathbf{a})).$$

We can get more information on ∇g_i by Corollary 1.5 and Lemma 1.6. The following Corollary says $\nabla g_i(T(\mathbf{a}))$ is invariant under shift, always perpendicular to $\mathbf{e}$, and equal to the negative of $\nabla g_{n-i}(T(\mathbf{a}^*))$. Furthermore if β_j's are symmetric, then $\nabla g_i(T(\mathbf{a}^R))$ is the reverse order of $\nabla g_i(T(\mathbf{a}))$.

Corollary 1.7 *Assume* $\mathbf{e}, \mathbf{a}, \mathbf{a}^R, \mathbf{a}^*$ *are the same as in Theorem 1.4, Definition 2 respectively. Then for scalars* σ, ω *and* $i = 1, 2, \ldots, n$

i. $\nabla g_i(T(\mathbf{a}+\sigma\mathbf{e})) = \nabla g_i(T(\mathbf{a}))$;

ii. $\nabla g_i(T(\mathbf{a})) \perp \mathbf{e}$;

iii. $\nabla g_i(T(\mathbf{a}^*)) = -\nabla g_{n-i}(T(\mathbf{a}))$;

iv. assume in addition $\beta_j = \beta_{n-j}$ *for* $j = 1, 2, \ldots, n-1$, *then*

$\nabla g_i(T(\mathbf{a}^R)) = [\nabla g_i(T(\mathbf{a}))]^R$.

Proof. Note that ∇g_i is a row vector, and matrix $D_a h(\mathbf{a})$ is the total derivative of h with respect to $\mathbf{a}$.

i. $\nabla_a\, g_i(T(\mathbf{a})) = \nabla_a\, g_i(T(\mathbf{a}+\sigma\mathbf{e})) = [\nabla g_i(T(\mathbf{a}+\sigma\mathbf{e}))]\, D_a(\mathbf{a}+\sigma\mathbf{e}) = \nabla g_i(T(\mathbf{a}+\sigma\mathbf{e}))$.

ii. $\nabla g_i(T(\mathbf{a}))\,\mathbf{e} = [\nabla g_i(T(\mathbf{a}+\sigma\mathbf{e}))]\,\mathbf{e} = \frac{d}{d\sigma} g_i(T(\mathbf{a}+\sigma\mathbf{e})) = \frac{d}{d\sigma} g_i(T(\mathbf{a})) = 0$.

Here is another proof using the normalization of $\mathbf{s}_i$'s,

$$\nabla g_i(T(\mathbf{a}))\,\mathbf{e} = \sum_{k=1}^{n} s_{i+1}(k)^2 - s_i(k)^2 = ||s_{i+1}||_2^2 - ||\mathbf{s}_i||_2^2 = 0.$$

iii. $\nabla_a\, g_{n-i}(T(\mathbf{a})) = \nabla_a\, g_i(T(\omega\mathbf{e}-\mathbf{a})) = [\nabla g_i(T(\omega\mathbf{e}-\mathbf{a}))]\, D_a(\omega\mathbf{e}-\mathbf{a}) = -\nabla g_i(T(\mathbf{a}^*))$.

iv. Consider $\hat{I}$ in Theorem 1.4 and $\beta_j = \beta_{n-j}$ for $j = 1, 2, \ldots, n-1$, then

$\nabla_a\, g_i(T(\mathbf{a})) = \nabla_a\, g_i(T(\hat{I}\mathbf{a})) = [\nabla g_i(T(\hat{I}\mathbf{a}))]\, D_a(\hat{I}\mathbf{a}) = [\nabla g_i(T(\mathbf{a}^R))]\,\hat{I} = [\nabla g_i(T(\mathbf{a}^R))]^R$.

□

1.6 Normalized Eigenvectors

Another surprising fact about tridiagonal matrices is that we have explicit formulae for their normalized eigenvectors in terms of eigenvalues. The following theorem was given by Paige in [8], as a corollary of Thompson and McEnteggert's result on adjugates [13]. We refer the readers to [9, Section 7.9] for more detail.

Before stating the result, we need the following notation

$$T_{j,k}(\mathbf{a}) := \operatorname{tridiag}\begin{pmatrix} & \beta_j & \cdots & \beta_{k-1} & \\ a(j) & \cdot & \cdots & \cdot & a(k) \\ & \beta_j & \cdots & \beta_{k-1} & \end{pmatrix} \qquad \text{for } j \le k,$$

$$\chi_{j,k}(\lambda) := \begin{cases} \det[\lambda I - T_{j,k}], & \text{if } j \le k; \\ 1, & \text{if } j > k. \end{cases}$$

$\chi'_{j,k}(\lambda)$ denotes the derivative of $\chi_{j,k}(\lambda)$ with respect to λ and $v(k)$ is the k-th entry of vector **v**.

Theorem 1.8 *Let $\{\lambda_i\}$ and $\{\mathbf{s_i}\}$ be eigenvalues and normalized eigenvectors of $T_{1,n}$. Then*

i. for $1 \le i \le n$ and $1 \le j \le k \le n$

$$\chi'_{1,n}(\lambda_i)s_i(j)s_i(k) = \chi_{1,j-1}(\lambda_i)\,\beta_j \cdots \beta_{k-1}\,\chi_{k+1,n}(\lambda_i);$$

ii. when λ_i is a simple eigenvalue (or $T_{1,n}$ unreduced),

$$s_i(j)^2 = \chi_{1,j-1}(\lambda_i)\,\chi_{j+1,n}(\lambda_i)/\chi'_{1,n}(\lambda_i).$$

Corollary 1.9 *For $i = 1, 2, \ldots, n$*

i. $\quad s_i(1)s_i(n)\chi'_{1,n}(\lambda_i) = \beta_1\beta_2\cdots\beta_{n-1};$

ii. $\quad s_i(1)^2\chi'_{1,n}(\lambda_i) = \chi_{2,n}(\lambda_i);$

iii. $\quad s_i(n)^2\chi'_{1,n}(\lambda_i) = \chi_{1,n-1}(\lambda_i);$

iv. $\quad \chi_{1,n-1}(\lambda_i)\chi_{2,n}(\lambda_i) = \beta_1^2\beta_2^2\cdots\beta_{n-1}^2.$

Proof.

i. Take $j = 1$ and $k = n$ in Theorem 1.8 (i).

ii. Take $j = k = 1$ in Theorem 1.8 (ii).

iii. Take $j = k = n$ in Theorem 1.8 (ii).

iv. By (i-iii)

$$\chi_{1,n-1}(\lambda_i)\chi_{2,n}(\lambda_i) = [s_i(1)s_i(n)\chi'_{1,n}(\lambda_i)]^2 = \prod_{k=1}^{n-1}\beta_k^2.$$

□

A matrix A is called *centrosymmetric* if it is symmetric with respect to both long diagonals, i.e.

$$A^T = A \qquad \text{and} \qquad \tilde{I}A\tilde{I} = A$$

where $\tilde{I}$ is defined in Theorem 1.4. Another way to characterize such a matrix $A = (a_{i,j})$ is

$$a_{i,j} = a_{j,i} = a_{n+1-j,n+1-i} = a_{n+1-i,n+1-j} \quad \text{for } i,j = 1,2,\ldots,n.$$

A centrosymmetric matrix can be split into two matrices of half the size such that each owns half of the original spectrum. Half of its eigenvectors are *symmetric*, i.e. $\mathbf{v}^R = \mathbf{v}$, and the other half are *skew symmetric*, i.e. $\mathbf{v}^R = -\mathbf{v}$. Here $\mathbf{v}^R$ is the reverse order of $\mathbf{v}$ defined in Definition 2 (i). We refer the readers to Cantoni and Butler's complete survey on centrosymmetric matrices [3].

Centrosymmetric tridiagonal matrices have the form

$$T_n = \text{tridiag}\begin{pmatrix} & \beta_1 & & \beta_2 & \cdots & \beta_2 & & \beta_1 & \\ a(1) & & a(2) & \cdot & \cdots & \cdot & a(2) & & a(1) \\ & \beta_1 & & \beta_2 & \cdots & \beta_2 & & \beta_1 & \end{pmatrix}.$$

Let $\{\lambda_i\}$ be the eigenvalues of T_n in ascending order and $\{\mathbf{s_i}\}$ be the corresponding normalized eigenvectors with $s_i(1) > 0$. Then $\mathbf{s_i}$'s are alternately symmetric and skew symmetric provided λ_i's are distinct. A complete picture of their behavior is stated below.

Even Case Suppose $n = 2m$. Define two matrices

$$T_m^{\pm} = \text{tridiag}\begin{pmatrix} & \beta_1 & \cdots & \beta_{m-2} & & \beta_{m-1} & \\ a(1) & \cdot & \cdots & \cdots & a(m-1) & & a(m) \pm \beta_m \\ & \beta_1 & \cdots & \beta_{m-2} & & \beta_{m-1} & \end{pmatrix}.$$

Let $\{\mu_i^{\pm}\}$ be the eigenvalues of $T_m^{\pm}$ in increasing order and $\{\mathbf{u_i^{\pm}}\}$ be the normalized eigenvectors with $u_i^{\pm}(1) > 0$. If λ_i's are distinct and $\beta_m > 0$, then

$$\lambda_{2k-1} = \mu_k^-, \qquad \mathbf{s_{2k-1}} = \frac{1}{\sqrt{2}}[\mathbf{u_k^-}, -(\mathbf{u_k^-})^R],$$

$$\lambda_{2k} = \mu_k^+, \qquad \mathbf{s_{2k}} = \frac{1}{\sqrt{2}}[\mathbf{u_k^+}, (\mathbf{u_k^+})^R]$$

for $k = 1,2,\ldots,m$. The situation is reversed if $\beta_m < 0$.

Odd Case Suppose $n = 2m+1$. Define

$$T_m^0 = \text{tridiag}\begin{pmatrix} & \beta_1 & \cdots & \beta_{m-1} & \\ a(1) & \cdot & \cdots & \cdot & a(m) \\ & \beta_1 & \cdots & \beta_{m-1} & \end{pmatrix},$$

and

$$T^{\dagger}_{m+1} = \text{tridiag}\begin{pmatrix} & \beta_1 & \cdots & \beta_{m-1} & & \sqrt{2}\beta_m & \\ a(1) & \cdot & \cdots & \cdot & a(m) & & a(m+1) \\ & \beta_1 & \cdots & \beta_{m-1} & & \sqrt{2}\beta_m & \end{pmatrix}.$$

Similarly define $\{\mu_i^0\}$, $\{\mu_i^{\dagger}\}$, $\{\mathbf{u}_i^0\}$, and $\{\mathbf{u}_i^{\dagger}\}$ as above. If λ_i's are distinct, then

$$\lambda_{2k} = \mu_k^0, \qquad \mathbf{s_{2k}} = \frac{1}{\sqrt{2}}[\mathbf{u_k^0}, 0, -(\mathbf{u_k^0})^R], \qquad \text{for } k = 1, 2, \ldots, m,$$

and $\qquad \lambda_{2k-1} = \mu_k^{\dagger}$,

$$\mathbf{s_{2k-1}} = \frac{1}{\sqrt{2}}(u_k^{\dagger}(1), \ldots, u_k^{\dagger}(m), \sqrt{2}u_k^{\dagger}(m+1), u_k^{\dagger}(m), \ldots, u_k^{\dagger}(1))$$

for $k = 1, 2, \ldots, m + 1$.

Notice that W_{2m+1} is centrosymmetric and the eigenvalues of W_m^0 interlace those of $W^{\dagger}_{m+1}$. Hence

$$g(W_{2m+1}) = g(W_m^0, W'^{\dagger}_{m+1}),$$

which can be estimated by Theorem 1.3.

Corollary 1.10 *For a centrosymmetric tridiagonal matrix T with positive subdiagonals,*

i. $\quad s_i(k) = (-1)^{n-i}s_i(n+1-k)$;

ii. $\quad s_i(j)^2 = \chi_{1,j-1}(\lambda_i)^2\beta_j\cdots\beta_{n-j} \,/\, |\chi'_{1,n}(\lambda_i)|$;

iii. $\quad s_i(1)^2 = \dfrac{\prod_{\nu=1}^{n-1}\beta_\nu}{\prod_{\substack{\nu=1\\ \nu\neq i}}^{n}|\lambda_i-\lambda_\nu|}$ *and* $s_i(2)^2 = \dfrac{(\lambda_i-a(1))^2\prod_{\nu=2}^{n-2}\beta_\nu}{\prod_{\substack{\nu=1\\ \nu\neq i}}^{n}|\lambda_i-\lambda_\nu|}$.

for $i, k = 1, 2, \ldots, n$ and $j = 1, 2, \ldots, [\frac{n+1}{2}]$.

Proof.

i. It follows from previous results on (skew) symmetry of eigenvectors. It can be proved by Theorem 1.8 as well. By centrosymmetry of T,

$$\chi'_{1,k-1}(\lambda_i) = \chi'_{n+2-k,n}(\lambda_i) \qquad \text{and} \qquad \chi'_{k+1,n}(\lambda_i) = \chi'_{1,n-k}(\lambda_i).$$

Hence $|s_i(k)| = |s_i(n+1-k)|$ by Theorem 1.8 (ii). Take $k = n+1-j$ in Theorem 1.8 (i),

$$\begin{aligned} \chi'_{1,n}(\lambda_i)s_i(j)s_i(n+1-j) &= \chi_{1,j-1}(\lambda_i)\,\beta_j\cdots\beta_{n-j}\,\chi_{n+2-j,n}(\lambda_i) \\ &= \chi_{1,j-1}(\lambda_i)^2\,\beta_j\cdots\beta_{j-1} > 0. \end{aligned} \tag{1.7}$$

Then

$$sign[s_i(j)s_i(n+1-j)] = sign[\chi'_{1,n}(\lambda_i)] = sign[\prod_{\substack{\nu=1\\ \nu\neq i}}^{n}(\lambda_i - \lambda_\nu)] = (-1)^{n-i}.$$

ii. Take absolute value of (1.7) and use (i).

iii. Take $j = 1$ and $j = 2$ in (ii).

□

Chapter 2

Extremal Matrix

In this chapter we devote ourselves to the extremal matrix

$$J_n(\mathbf{w}_1) = \mathrm{tridiag}\begin{pmatrix} & 1 & & 1 & \cdots & 1 & & 1 & \\ \omega & & 0 & \cdot & \cdots & \cdot & 0 & & \omega \\ & 1 & & 1 & \cdots & 1 & & 1 & \end{pmatrix}.$$

We will discuss its eigenvalues, eigenvectors, and gap in full detail. It deserves our attention because $g_{n-1}(J_n(\mathbf{w}_1))$ minimizes our objective (1.4) for large enough ω. But more important is that we use this gap to eliminate the other separations and solve (1.4).

2.1 Eigenvalues and Eigenvectors

Suppose

$$J_n(\mathbf{w}_1)\mathbf{v}(\lambda) = \lambda \mathbf{v}(\lambda)$$

with $\mathbf{v}(\lambda) = (\nu_1(\lambda), \nu_2(\lambda), \ldots, \nu_n(\lambda))$, then

$$\begin{aligned} (\omega - \lambda)\nu_1(\lambda) + \nu_2(\lambda) &= 0, \\ \nu_{k-1}(\lambda) - \lambda\nu_k(\lambda) + \nu_{k+1}(\lambda) &= 0, \qquad k = 2, 3, \ldots, n-1, \\ \nu_{n-1}(\lambda) + (\omega - \lambda)\nu_n(\lambda) &= 0. \end{aligned} \tag{2.1}$$

If we set $\nu_0(\lambda) = \omega$ and $\nu_1(\lambda) = 1$, then we can extend the three-term recurrence

$$\nu_{k+1}(\lambda) = \lambda\, \nu_k(\lambda) - \nu_{k-1}(\lambda). \tag{2.2}$$

to $k = 1, 2, \ldots, n-1$.

Recall that the Chebyshev polynomials of second kind satisfy the same recurrence relation. To be more precise, let

$$U_{k-1}(x) = \begin{cases} \frac{\sin(k\cos^{-1}x)}{\sin(\cos^{-1}x)} & |x| \le 1; \\ \frac{\sinh(k\cosh^{-1}x)}{\sinh(\cosh^{-1}x)} & |x| > 1; \end{cases}$$

for $k = 0, 1, 2, \ldots$. Then

$$U_{k+1}(x) = 2xU_k(x) - U_{k-1}(x), \tag{2.3}$$

for $k = 0, 1, 2, \ldots$, with $U_{-1}(x) = 0$, $U_0(x) = 1$, $U_1(x) = 2x$, etc. Observe that

$$U_0(\frac{\lambda}{2}) = 1,\ U_1(\frac{\lambda}{2}) = \lambda,\ U_2(\frac{\lambda}{2}),\ U_3(\frac{\lambda}{2}),\ \ldots,$$

and

$$U_{-1}(\frac{\lambda}{2}) = 0,\ U_0(\frac{\lambda}{2}) = 1,\ U_1(\frac{\lambda}{2}),\ U_2(\frac{\lambda}{2}),\ \ldots,$$

are two linearly independent solutions of (2.2), so the sequence $\{\nu_i(\lambda) | i = 0, 1, \ldots, n\}$ can be expressed as their linear combination. Indeed

$$\nu_{k+1}(\lambda) = U_k(\frac{\lambda}{2}) - \omega U_{k-1}(\frac{\lambda}{2}) \qquad \text{for } k = 0, 1, \ldots, n-1. \tag{2.4}$$

Notice that the Chebyshev polynomials of first kind $T_k(x)$ obey (2.3) too, but have different initial conditions

$$T_0(x) = 1,\ T_1(x) = x,\ T_2(x) = 2x^2 - 1, \text{ etc.}$$

Therefore we can have different expressions for ν_k, for example

$$\begin{aligned} \nu_{k+1}(\lambda) &= \frac{2\omega}{\lambda} T_k(\frac{\lambda}{2}) + (1 - \frac{2\omega}{\lambda}) U_k(\frac{\lambda}{2}) \\ &= T_k(\frac{\lambda}{2}) + (\frac{\lambda}{2} - \omega) U_{k-1}(\frac{\lambda}{2}) \\ &= \frac{4\omega - 2\lambda}{4 - \lambda^2} T_k(\frac{\lambda}{2}) + \frac{4 - 2\lambda\omega}{4 - \lambda^2} T_{k-1}(\frac{\lambda}{2}) \end{aligned}$$

for $k = 0, 1, \ldots, n-1$. As a matter of fact, we can solve the difference equation(2.2) directly. $(\frac{\lambda + \sqrt{\lambda^2 - 4}}{2})^k$ and $(\frac{\lambda - \sqrt{\lambda^2 - 4}}{2})^k$ are two linearly independent solutions if $\lambda \neq \pm 2$. Thus

$$\nu_k(\lambda) = \frac{1}{2}(\omega + \frac{2 - \lambda\omega}{\sqrt{\lambda^2 - 4}})(\frac{\lambda + \sqrt{\lambda^2 - 4}}{2})^k + \frac{1}{2}(\omega - \frac{2 - \lambda\omega}{\sqrt{\lambda^2 - 4}})(\frac{\lambda - \sqrt{\lambda^2 - 4}}{2})^k$$

for $k = 0, 1, \ldots, n-1$.

Clearly (2.4) is the simplest form. Notice that we have not used (2.1) yet, which gives us the eigenvalue equation. Hence we can solve for all the eigenvalues, and then find all the eigenvectors by (2.4). For centrosymmetric $J_n(\mathbf{w_1})$, however, the spectrum can be split by the technique in Section 1.6. Instead of original matrix, we then deal with two matrices of half the size.

We first locate the eigenvalue $\{\lambda_i\}$ of $J_n(\mathbf{w_1})$ by Gershgorin's Disk Theorem, which says $\lambda_i \in [-2,2] \cup [\omega - 1, \omega + 1]$ for all i's. For an irreducible matrix, a boundary point of the Gershgorin disks can be an eigenvalue only if every Gershgorin circle lies on it [5, Theorem 6.2.26]. Thus when $\omega > 3$,

$$-2 < \lambda_1 < \cdots < \lambda_{n-2} < 2 < \omega - 1 < \lambda_{n-1} < \lambda_n < \omega + 1. \tag{2.5}$$

We assume this case in the sequel.

Even Case Suppose $n = 2m$ and

$$J_m^{\pm} := \text{tridiag}\begin{pmatrix} & 1 & & 1 & \cdots & 1 & & 1 & \\ \omega & & 0 & \cdot & \cdots & \cdot & 0 & & \pm 1 \\ & 1 & & 1 & \cdots & 1 & & 1 & \end{pmatrix},$$

then $\{\lambda_{2k-1}\}_{k=1}^m$ constitutes the spectrum of J_m^- and $\{\lambda_{2k}\}_{k=1}^m$ constitutes that of J_m^+ while

$$\mathbf{u}(\lambda_i) = (\nu_1(\lambda_i), \nu_2(\lambda_i), \ldots, \nu_m(\lambda_i))$$

is the corresponding eigenvector.

Using the last equation in system $J_m^{\pm}\mathbf{u}(\lambda) = \lambda\mathbf{u}(\lambda)$, we have

$$\nu_{m-1}(\lambda) + (\pm 1 - \lambda)\nu_m(\lambda) = 0,$$

$$\begin{aligned} \pm\nu_m(\lambda) &= \lambda\nu_m(\lambda) - \nu_{m-1}(\lambda) = \nu_{m+1}(\lambda), \\ \pm[U_{m-1}(\frac{\lambda}{2}) - \omega U_{m-2}(\frac{\lambda}{2})] &= U_m(\frac{\lambda}{2}) - \omega U_{m-1}(\frac{\lambda}{2}), \\ \pm U_{m-1}(\frac{\lambda}{2}) - U_m(\frac{\lambda}{2}) &= \omega[\pm U_{m-2}(\frac{\lambda}{2}) - U_{m-1}(\frac{\lambda}{2})] \end{aligned} \tag{2.6}$$

by (2.2) and (2.4). As expected, the eigenvalue λ is a zero of a polynomial of degree m. In fact (2.6) is nothing but the characteristic equation $det[\lambda I - J_m^{\pm}] = 0$.

Suppose λ is λ_{n-1} or λ_n, then $\frac{\lambda}{2} > 1$ by (2.5). So we can change variable $\frac{\lambda}{2} = \cosh\phi$, where $\phi \neq 0$, in (2.6) to get

$$\pm U_{m-1}(\cosh\phi) - U_m(\cosh\phi) = \omega[\pm U_{m-2}(\cosh\phi) - U_{m-1}(\cosh\phi)],$$

$$\pm \sinh m\phi - \sinh(m+1)\phi = \omega[\pm \sinh(m-1)\phi - \sinh m\phi],$$

$$\begin{cases} (+): & -2\sinh\frac{\phi}{2}\,\cosh(m+\frac{1}{2})\phi = -2\omega\sinh\frac{\phi}{2}\,\cosh(m-\frac{1}{2})\phi, \\ (-): & -2\sinh(m+\frac{1}{2})\phi\,\cosh\frac{\phi}{2} = -2\omega\sinh(m-\frac{1}{2})\phi\,\cosh\frac{\phi}{2}, \end{cases}$$

$$\begin{cases} (+): & \cosh(m+\frac{1}{2})\phi = \omega\cosh(m-\frac{1}{2})\phi, \\ (-): & \sinh(m+\frac{1}{2})\phi = \omega\sinh(m-\frac{1}{2})\phi. \end{cases} \tag{2.7}$$

Again consider $t = e^{\phi}$, then $t > 0$, $t \neq 1$,

$$\cosh \ell\phi = \frac{1}{2}(e^{\ell\phi} + e^{-\ell\phi}) = \frac{1}{2}(t^{\ell} + \frac{1}{t^{\ell}}),$$

and

$$\sinh \ell\phi = \frac{1}{2}(e^{\ell\phi} - e^{-\ell\phi}) = \frac{1}{2}(t^{\ell} - \frac{1}{t^{\ell}}).$$

Hence (2.7) can be further simplified to

$$(+): \quad \omega = \frac{t^{m+\frac{1}{2}} + t^{-(m+\frac{1}{2})}}{t^{m-\frac{1}{2}} + t^{-(m-\frac{1}{2})}} = \frac{t^{2m+1}+1}{t^{2m}+t} = \frac{t^{2m} - t^{2m-1} + \cdots - t + 1}{t^{2m-1} - t^{2m-2} + \cdots - t^2 + t}, \tag{2.8}$$

$$(-): \quad \omega = \frac{t^{m+\frac{1}{2}} - t^{-(m+\frac{1}{2})}}{t^{m-\frac{1}{2}} - t^{-(m-\frac{1}{2})}} = \frac{t^{2m+1}-1}{t^{2m}-t} = \frac{t^{2m} + t^{2m-1} + \cdots + t + 1}{t^{2m-1} + t^{2m-2} + \cdots + t^2 + t}. \tag{2.9}$$

When λ is one of $\lambda_1, \ldots, \lambda_{n-2}$, $\frac{\lambda}{2} \in (-1, 1)$ by (2.5). We can change variable $\lambda = 2\cos\varphi = z + \frac{1}{z}$, where $z = e^{i\varphi}$ and $\varphi \in (0, \pi)$. Notice that $\sin\varphi \neq 0$ for all φ in $(0, \pi)$, thus z is not a real number. The same computation shows that z satisfies (2.8) or (2.9) as well.

Both (2.8) and (2.9) have $2m$ roots. Replacing t by $\frac{1}{t}$ in (2.8) and (2.9), we get the same equations. Therefore their roots come in pairs, i.e. t and $\frac{1}{t}$. However we recover the same eigenvalue λ from both t and $\frac{1}{t}$.

Hence (2.8) has a pair of positive roots corresponding to λ_n, and the other zeros on unit circle corresponding to $\lambda_2, \lambda_4, \ldots, \lambda_{n-2}$. Similarly two positive zeros of (2.9) give λ_{n-1} and the other complex roots give $\lambda_1, \lambda_3, \ldots, \lambda_{n-3}$.

Odd Case Suppose $n = 2m + 1$. The

$$J_m^0 := \operatorname{tridiag}\begin{pmatrix} & 1 & & 1 & \cdots & 1 & \\ \omega & & 0 & \cdot & \cdots & \cdot & 0 \\ & 1 & & 1 & \cdots & 1 & \end{pmatrix}$$

has eigenvalues $\{\lambda_{2k}\}_{k=1}^{m}$, which satisfy

$$\nu_{m-1}(\lambda) - \lambda\nu_m(\lambda) = 0.$$

Thus by (2.2) and (2.4)

$$U_m(\frac{\lambda}{2}) - \omega U_{m-1}(\frac{\lambda}{2}) = \nu_{m+1}(\lambda) = 0.$$

Change variable

$$\begin{cases} \lambda = 2\cosh\phi = e^{\phi} + e^{-\phi} = t + \frac{1}{t}, & \text{if } \lambda > 1; \\ \lambda = 2\cos\varphi = e^{i\varphi} + e^{-i\varphi} = t + \frac{1}{t}, & \text{if } |\lambda| < 1; \end{cases} \tag{2.10}$$

then

$$\omega = \frac{U_m(\frac{\lambda}{2})}{U_{m-1}(\frac{\lambda}{2})} = \frac{t^{2m+2} - 1}{t^{2m+1} - t} = \frac{t^{2m} + t^{2m-2} + \cdots + t^2 + 1}{t^{2m-1} + t^{2m-3} + \cdots + t^3 + t}. \tag{2.11}$$

(2.11) has $2m$ zeros which are in pairs. λ_{n-1} comes from the only pair of positive roots, and $\lambda_2, \lambda_4, \ldots, \lambda_{n-3}$ come from the other $m-1$ pairs of complex roots.

In the other hand

$$J_{m+1}^{\dagger} := \text{tridiag}\begin{pmatrix} & 1 & & 1 & \cdots & 1 & & \sqrt{2} & \\ \omega & & 0 & \cdot & \cdots & \cdot & 0 & & 0 \\ & 1 & & 1 & \cdots & 1 & & \sqrt{2} & \end{pmatrix}$$

has eigenvalues $\{\lambda_{2k-1}\}_{k=1}^{m+1}$ and eigenvectors

$$(\nu_1(\lambda_{2k-1}), \ldots, \nu_m(\lambda_{2k-1}), \frac{1}{\sqrt{2}}\nu_{m+1}(\lambda_{2k-1})).$$

The eigenvalue equation is

$$\sqrt{2}\nu_m(\lambda) - \lambda\frac{1}{\sqrt{2}}\nu_{m+1}(\lambda) = 0.$$

Thus by (2.2) and (2.4)

$$\nu_m(\lambda) = \lambda\nu_{m+1}(\lambda) - \nu_m(\lambda) = \nu_{m+2}(\lambda),$$

$$U_{m-1}(\frac{\lambda}{2}) - \omega U_{m-2}(\frac{\lambda}{2}) = U_{m+1}(\frac{\lambda}{2}) - \omega U_m(\frac{\lambda}{2}),$$

$$\omega\,[U_m(\frac{\lambda}{2}) - U_{m-2}(\frac{\lambda}{2})] = U_{m+1}(\frac{\lambda}{2}) - \omega U_{m-1}(\frac{\lambda}{2}),$$

Using (2.10), we have

$$\omega = \frac{U_{m+1}(\frac{\lambda}{2}) - U_{m-1}(\frac{\lambda}{2})}{U_m(\frac{\lambda}{2}) - U_{m-2}(\frac{\lambda}{2})} = \frac{t^{m+1} + t^{-(m+1)}}{t^m + t^{-m}} = \frac{t^{2m+2} + 1}{t^{2m+1} + t}. \tag{2.12}$$

(2.12) has $2m+2$ zeros and they comes in pairs as well. The only positive pair gives λ_n, and the other m complex pairs give $\lambda_1, \lambda_3, \ldots, \lambda_{n-2}$.

We summarize as follows. Let τ and τ' be the smallest positive roots of $p(t) = \omega$ and $q(t) = \omega$ respectively, where

$$p(t) := \frac{t^{n+1} + 1}{t^n + t} \tag{2.13}$$

and

$$q(t) := \frac{t^{n+1} - 1}{t^n - t}. \tag{2.14}$$

Then

$$\lambda_n = \tau + \frac{1}{\tau} \qquad \text{and} \qquad \lambda_{n-1} = \tau' + \frac{1}{\tau'}. \tag{2.15}$$

Since $p(t)$ and $q(t)$ are negative in $(-\infty, 0)$, decrease from $+\infty$ to 1 in $(0, 1)$, and increase from 1 to $+\infty$ in $[1, +\infty)$, each function hits ω (> 3) exactly twice. In fact τ and $\frac{1}{\tau}$ are the only real roots of $p(t) = \omega$, and so are τ' and $\frac{1}{\tau'}$ of $q(t) = \omega$.

2.2 Asymptotic Expansions

In this section we compute the asymptotic expansions of λ_n and λ_{n-1}. The tool is the Hensel iteration in the power series domain $\mathbf{R}[[x]]$. Let $f(y)$ be a polynomial with coefficients in $\mathbf{R}[[x]]$ and y_0 in $\mathbf{R}$ be an $O(x)$ approximation to a root of $f(y)$, i.e. $y = y_0$ is a solution to $f(y) = 0$ when $x = 0$. Suppose $f'(y_0) := \frac{df}{dy}(y_0) \neq 0$ when $x = 0$, then the sequence of iterations defined by

$$y_k := y_{k-1} - \frac{f(y_{k-1})}{f'(y_0)} \qquad (\text{mod } x^{k+1}) \qquad k = 1, 2, \ldots \tag{2.16}$$

has the property that y_k is an $O(x^{k+1})$ approximation to y. This is the Hensel iteration, which converges linearly.

Under the same hypotheses we have the well known Newton iteration

$$y_k := y_{k-1} - \frac{f(y_{k-1})}{f'(y_{k-1})} \qquad (\text{mod } x^{2^k}) \qquad k = 1, 2, \ldots,$$

which has the property that y_k is an $O(x^{2^k})$ approximation to y. The quadratically convergent Newton iteration is superior to the Hensel iteration in general. However each step in Hensel iteration is less expensive since no recomputation of f' is required. Therefore Hensel iteration seems cheaper if only a few terms in power series are needed. This is the reason why we use (2.16) in the following computation.

We are ready to find the asymptotic expansion of $\lambda_n(\omega)$. First we convert λ_n to a power series in ϵ near $\epsilon = 0$ by setting $\epsilon = \frac{1}{\omega}$. Recall λ_n comes from $p(t) - \omega = 0$, which now becomes

$$\frac{t^{n+1}+1}{t^n+t} - \frac{1}{\epsilon} = 0.$$

Therefore we consider

$$f(t) = \epsilon(t^{n+1}+1) - (t^n + t).$$

and its smallest positive root τ. We apply the Hensel iteration on f to expand τ as a power series of ϵ.

To obtain the initial value t_0, consider $\epsilon = 0$. Then $f(t) = -t(t^{n-1}+1) = 0$, and $t_0 = 0$ will be the appropriate guess for the smallest positive root of f. By (2.16)

$$t_1 = t_0 - \frac{f(t_0)}{f'(t_0)} \pmod{\epsilon^2} = \epsilon.$$

Since

$$f(t_1) = \epsilon(\epsilon^{n+1}+1) - (\epsilon^n + \epsilon) = \epsilon^{n+2} - \epsilon^n,$$

t_1 is an $O(\epsilon^n)$ approximation to τ, which is far more promising than t_0. Hence it is better to start the Hensel iteration from t_1 so that each iteration improves $n-1$ terms. More precisely let $t_2, t_3, \ldots$ be the successive approximations by (2.16), then

$$\Delta t_k = -\frac{f(t_k)}{f'(t_1)} \qquad (\mathrm{mod}\ \epsilon^{1+(n-1)(k+1)}), \tag{2.17}$$

for $k \geq 1$, where Δ is the forward difference.

Observe that

$$f'(t_1) = \epsilon(n+1)t_1^n - nt_1^{n-1} - 1 = -[1 + n\epsilon^{n-1} - (n+1)\epsilon^{n+1}],$$

and

$$\frac{-1}{f'(t_1)} = 1 - [n\epsilon^{n-1} - (n+1)\epsilon^{n+1}] + [n\epsilon^{n-1} - (n+1)\epsilon^{n+1}]^2 + \cdots = 1 + O(\epsilon^{n-1}).$$

Thus

$$\begin{aligned}
\Delta t_1 &= f(t_1)((1+O(\epsilon^{n-1})) = (\epsilon^{n+2} - \epsilon^n)(1+O(\epsilon^{n-1})) \equiv -\epsilon^n + \epsilon^{n+2} \pmod{\epsilon^{2n-1}}, \\
t_2 &= t_1 + \Delta t_1 = \epsilon - \epsilon^n + \epsilon^{n+2}, \\
f(t_2) &= \epsilon(t_2^{n+1}+1) - (t_2^n + t_2) = \epsilon[(t_1+\Delta t_1)^{n+1} + 1] - [(t_1+\Delta t_1)^n + (t_1+\Delta t_1)]
\end{aligned}$$

$$
\begin{aligned}
&= \epsilon\,[t_1^{n+1} + (n+1)\,t_1^n \Delta t_1 + \binom{n+1}{2} t_1^{n-1} \Delta t_1^2 + O(\epsilon^{4n-2}) + 1] \\
&\quad -[t_1^n + n t_1^{n-1} \Delta t_1 + \binom{n}{2} t_1^{n-2} \Delta t_1^2 + O(\epsilon^{4n-3}) + t_1 + \Delta t_1] \\
&= \epsilon\,(t_1^{n+1} + 1) - (t_1^n + t_1) + t_1^{n-1} \Delta t_1 [(n+1)\epsilon\, t_1 - n] \\
&\quad + \frac{n}{2} t_1^{n-2} \Delta t_1^2 [(n+1)\epsilon\, t_1 - (n-1)] - \Delta t_1 + O(\epsilon^{4n-3}) \\
&= f(t_1) - \Delta t_1 + \epsilon^{n-1}(-\epsilon^n + \epsilon^{n+2})[(n+1)\epsilon^2 - n] \\
&\quad + \frac{n}{2} \epsilon^{n-2} (-\epsilon^n + \epsilon^{n+2})^2 [(n+1)\epsilon^2 - (n-1)] + O(\epsilon^{4n-3}) \\
&= n\epsilon^{2n-1} - (2n+1)\epsilon^{2n+1} + (n+1)\epsilon^{2n+3} - \frac{n(n-1)}{2}\epsilon^{3n-2} \\
&\quad + \frac{n(3n-1)}{2}\epsilon^{3n} - \frac{n(3n+1)}{2}\epsilon^{3n+2} + \frac{n(n+1)}{2}\epsilon^{3n+4} + O(\epsilon^{4n-3}), \\
\Delta t_2 &= -\frac{f(t_2)}{f'(t_1)} = [n\epsilon^{2n-1} - (2n+1)\epsilon^{2n+1} + (n+1)\epsilon^{2n+3} + O(\epsilon^{3n-2})]\,[1 + O(\epsilon^{n-1})] \\
&\equiv n\epsilon^{2n-1} - (2n+1)\epsilon^{2n+1} + (n+1)\epsilon^{2n+3} \qquad (\text{mod } \epsilon^{3n-2}), \\
t_3 &= t_2 + \Delta t_2 = \epsilon - \epsilon^n + \epsilon^{n+2} + n\epsilon^{2n-1} - (2n+1)\epsilon^{2n+1} + (n+1)\epsilon^{2n+3}, \\
f(t_3) &= \epsilon\,(t_3^{n+1} + 1) - (t_3^n + t_3) = \epsilon\,[(t_2 + \Delta t_2)^{n+1} + 1] - [(t_2 + \Delta t_2)^n + (t_2 + \Delta t_2)] \\
&= \epsilon\,(t_2^{n+1} + 1) - (t_2^n + t_2) + t_2^{n-1} \Delta t_2 [(n+1)\epsilon\, t_2 - n] - \Delta t_2 + O(\epsilon^{5n-4}) \\
&= f(t_2) - \Delta t_2 + (\epsilon - \epsilon^n + \epsilon^{n+2})^{n-1} [n\epsilon^{2n-1} - (2n+1)\epsilon^{2n+1} + (n+1)\epsilon^{2n+3}] \\
&\qquad \cdot [-n + (n+1)(\epsilon^2 - \epsilon^{n+1} + \epsilon^{n+3})] + O(\epsilon^{5n-4}) \\
&= -\frac{n(n-1)}{2}\epsilon^{3n-2} + \frac{n(3n-1)}{2}\epsilon^{3n} - \frac{n(3n+1)}{2}\epsilon^{3n+2} + \frac{n(n+1)}{2}\epsilon^{3n+4} + O(\epsilon^{4n-3}) \\
&\quad - n^2\epsilon^{3n-2} + n(3n+2)\epsilon^{3n} - (n+1)(3n+1)\epsilon^{3n+2} + (n+1)^2\epsilon^{3n+4} + O(\epsilon^{4n-3}) \\
&= -\frac{n(3n-1)}{2}\epsilon^{3n-2} + \frac{3n(3n+1)}{2}\epsilon^{3n} - \frac{(3n+1)(3n+2)}{2}\epsilon^{3n+2} \\
&\quad + \frac{(n+1)(3n+2)}{2}\epsilon^{3n+4} + O(\epsilon^{4n-3}), \\
\Delta t_3 &= -\frac{f(t_3)}{f'(t_1)} = f(t_3)\,[1 + O(\epsilon^{n-1})] \\
&\equiv -\frac{n(3n-1)}{2}\epsilon^{3n-2} + \frac{3n(3n+1)}{2}\epsilon^{3n} - \frac{(3n+1)(3n+2)}{2}\epsilon^{3n+2} \\
&\quad + \frac{(n+1)(3n+2)}{2}\epsilon^{3n+4} \qquad (\text{mod } \epsilon^{4n-3}), \\
t_4 &= \epsilon - \epsilon^n + \epsilon^{n+2} + n\epsilon^{2n-1} - (2n+1)\epsilon^{2n+1} + (n+1)\epsilon^{2n+3} - \frac{n(3n-1)}{2}\epsilon^{3n-2} \\
&\quad + \frac{3n(3n+1)}{2}\epsilon^{3n} - \frac{(3n+1)(3n+2)}{2}\epsilon^{3n+2} + \frac{(n+1)(3n+2)}{2}\epsilon^{3n+4}.
\end{aligned}
$$

Since t_4 is an $O(\epsilon^{4n-3})$ approximation to the root τ,

$$\tau = t_4 + O(\epsilon^{4n-3}).$$

Recall that $\lambda_n = \tau + \frac{1}{\tau}$, so the power series of $\frac{1}{\tau}$ is needed as well. Notice that $\frac{1}{\tau}$ is in fact the largest root of f. Hence we can repeat Hensel iteration with appropriate initial guess to expand $\frac{1}{\tau}$. However it is easier to invert it directly

$$\begin{aligned}
&\frac{1}{\tau} = [t_4 + O(\epsilon^{4n-3})]^{-1} \\
= \quad & \frac{1}{\epsilon}[1 - \epsilon^{n-1} + \epsilon^{n+1} + n\epsilon^{2n-2} - (2n+1)\epsilon^{2n} + (n+1)\epsilon^{2n+2} \\
& \quad -\frac{n(3n-1)}{2}\epsilon^{3n-3} + O(\epsilon^{3n-1})]^{-1} \\
= \quad & \frac{1}{\epsilon}\{1 + [\epsilon^{n-1} - \epsilon^{n+1} - n\epsilon^{2n-2} + (2n+1)\epsilon^{2n} - (n+1)\epsilon^{2n+2} + \frac{n(3n-1)}{2}\epsilon^{3n-3}] \\
& \quad +[\epsilon^{n-1} - \epsilon^{n+1} - n\epsilon^{2n-2}]^2 + \epsilon^{3n-3} + O(\epsilon^{3n-1})\} \\
= \quad & \frac{1}{\epsilon}\{1 + \epsilon^{n-1} - \epsilon^{n+1} - (n-1)\epsilon^{2n-2} + (2n-1)\epsilon^{2n} - n\epsilon^{2n+2} \\
& \quad +\frac{(n-1)(3n-2)}{2}\epsilon^{3n-3} + O(\epsilon^{3n-1})\} \\
= \quad & \frac{1}{\epsilon} + \epsilon^{n-2} - \epsilon^{n} - (n-1)\epsilon^{2n-3} + (2n-1)\epsilon^{2n-1} - n\epsilon^{2n+1} \\
& \quad +\frac{(n-1)(3n-2)}{2}\epsilon^{3n-4} + O(\epsilon^{3n-2}),
\end{aligned} \tag{2.18}$$

by the formula of geometric series $\frac{1}{1-r} = 1 + r + r^2 + \cdots$. Finally by (2.15) we have

$$\begin{aligned}
&\lambda_n = \tau + \frac{1}{\tau} \\
= \quad & \frac{1}{\epsilon} + \epsilon + \epsilon^{n-2} - 2\epsilon^{n} + \epsilon^{n+2} - (n-1)\epsilon^{2n-3} + (3n-1)\epsilon^{2n-1} \\
& \quad -(3n+1)\epsilon^{2n+1} + (n+1)\epsilon^{2n+3} + \frac{(n-1)(3n-2)}{2}\epsilon^{3n-4} + O(\epsilon^{3n-2}) \\
= \quad & (\omega + \frac{1}{\omega}) + \frac{(\omega - \frac{1}{\omega})^2}{\omega^n} - \frac{n-1}{\omega^{2n-3}} + \frac{3n-1}{\omega^{2n-1}} - \frac{3n+1}{\omega^{2n+1}} + \frac{n+1}{\omega^{2n+3}} \\
& \quad +\frac{(n-1)(3n-2)}{2\omega^{3n-4}} + O(\frac{1}{\omega^{3n-2}}).
\end{aligned} \tag{2.19}$$

Similarly we can get the asymptotic expansion for $\lambda_{n-1}(\omega)$. This time we consider the smallest root τ' of function

$$h(t) = \epsilon\,(t^{n+1} - 1) - t^n + t.$$

The initial guess $t'_0 = 0$ and $t'_1 = \epsilon$ are the same. Then

$$\Delta t'_1 = \epsilon^n - \epsilon^{n+2},$$

$$\Delta t'_2 = n\epsilon^{2n-1} - (2n+1)\epsilon^{2n+1} + (n+1)\epsilon^{2n+3},$$

$$\Delta t'_3 = \frac{n(3n-1)}{2}\epsilon^{3n-2} - \frac{3n(3n+1)}{2}\epsilon^{3n} + \frac{(3n+1)(3n+2)}{2}\epsilon^{3n+2} - \frac{(n+1)(3n+2)}{2}\epsilon^{3n+4}$$

by Hensel iteration. It follows that

$$\tau' = \epsilon + \epsilon^n - \epsilon^{n+2} + n\epsilon^{2n-1} - (2n+1)\epsilon^{2n+1} + (n+1)\epsilon^{2n+3} + \frac{n(3n-1)}{2}\epsilon^{3n-2} + O(\epsilon^{3n}) \quad (2.20)$$

and

$$\frac{1}{\tau'} = \frac{1}{\epsilon} - \epsilon^{n-2} + \epsilon^n - (n-1)\epsilon^{2n-3} + (2n-1)\epsilon^{2n-1} - n\epsilon^{2n+1} - \frac{(n-1)(3n-2)}{2}\epsilon^{3n-4} + O(\epsilon^{3n-2}). \quad (2.21)$$

Therefore by (2.15)

$$\begin{aligned} \lambda_{n-1} &= \tau' + \frac{1}{\tau'} \\ &= \frac{1}{\epsilon} + \epsilon - \epsilon^{n-2} + 2\epsilon^n - \epsilon^{n+2} - (n-1)\epsilon^{2n-3} + (3n-1)\epsilon^{2n-1} \\ &\quad - (3n+1)\epsilon^{2n+1} + (n+1)\epsilon^{2n+3} - \frac{(n-1)(3n-2)}{2}\epsilon^{3n-4} + O(\epsilon^{3n-2}) \\ &= (\omega + \frac{1}{\omega}) - \frac{(\omega - \frac{1}{\omega})^2}{\omega^n} - \frac{n-1}{\omega^{2n-3}} + \frac{3n-1}{\omega^{2n-1}} - \frac{3n+1}{\omega^{2n+1}} + \frac{n+1}{\omega^{2n+3}} \\ &\quad - \frac{(n-1)(3n-2)}{2\omega^{3n-4}} + O(\frac{1}{\omega^{3n-2}}). \end{aligned} \quad (2.22)$$

We used the modulo $\epsilon^{1+(n-1)(k+1)}$ representation in the iteration (2.17). It seems that we implicitly assume $n+2 < 2n-1$ in Δt_1 and $2n+3 < 3n-2$ in Δt_2, etc. However these assumptions are not required for a legitimate iteration. The reason is that the extra error terms won't affect the order of approximation. Similarly for (2.18) to (2.22), several terms overlap to each other when $2n+3 \geq 3n-4$, but the validity of the expansions remains. We conclude that (2.19) and (2.22) hold for $n \geq 2$ and

Theorem 2.1 *For $n \geq 2$, the matrix $J_n(\mathbf{w}_1)$ has two dominant eigenvalues that satisfy*

$$\begin{aligned} \lambda_n - \lambda_{n-1} &= \frac{2(\omega - \frac{1}{\omega})^2}{\omega^n} + \frac{(n-1)(3n-2)}{\omega^{3n-4}} + O(\frac{1}{\omega^{3n-2}}) \\ &\geq 2(\omega - \frac{1}{\omega})^2/\omega^n \qquad \textit{as} \quad \omega \to \infty. \end{aligned}$$

Let's look at two cases when n is small. We can compute the eigenvalues directly from the characteristic polynomial. Indeed

$$J_2(\mathbf{w_1}) = \begin{pmatrix} \omega & 1 \\ 1 & \omega \end{pmatrix}$$

has eigenvalues $\omega \pm 1$ and

$$\lambda_2 - \lambda_1 = 2 = \frac{2(\omega - \frac{1}{\omega})^2}{\omega^2} + \frac{4}{\omega^2} + O(\frac{1}{\omega^4}).$$

$J_3(\mathbf{w_1})$ has eigenvalues

$$\lambda_1 = \frac{1}{2}(\omega - \sqrt{\omega^2 + 8}), \quad \lambda_2 = \omega, \quad \text{and } \lambda_3 = \frac{1}{2}(\omega + \sqrt{\omega^2 + 8})$$

$$\begin{aligned} \text{with} \qquad \lambda_3 - \lambda_2 &= \frac{1}{2}(\sqrt{\omega^2 + 8} - \omega) && (2.23) \\ &= \frac{\omega}{2}(\sqrt{1 + \frac{8}{\omega^2}} - 1) \\ &= \frac{\omega}{2}[\frac{4}{\omega^2} - \frac{8}{\omega^4} + \frac{32}{\omega^6} + O(\frac{1}{\omega^8})] \\ &= \frac{2}{\omega} - \frac{4}{\omega^3} + \frac{16}{\omega^5} + O(\frac{1}{\omega^7}). \\ &= \frac{2(\omega - \frac{1}{\omega})^2}{\omega^3} + \frac{14}{\omega^5} + O(\frac{1}{\omega^7}). \end{aligned}$$

2.3 Bounds for $\lambda_n - \lambda_{n-1}$

Although (2.19), (2.22) and Theorem 2.1 are asymptotic, there are precise bounds for λ_n, λ_{n-1} and $\lambda_n - \lambda_{n-1}$. We need the following lemma, whose assertions are suggested by the expansions of (2.18) and (2.21).

Lemma 2.2 i. *Suppose $n \geq 3$ and $\omega > 3$, then $\omega + \frac{2}{\omega^{n-1}} < \frac{1}{\tau} < \omega + \frac{1}{\omega^{n-2}}$.*

ii. *Suppose $n \geq 4$ and $\omega > 3$, then $\omega - \frac{1}{\omega^{n-2}} < \frac{1}{\tau'} < \omega - \frac{2}{\omega^{n-1}}$.*

Proof.

i. Recall that $\frac{1}{\tau}$ is the largest zero of $f(t)$ or $p(t) - \omega$, where p is defined by (2.13). For $\omega > 1$, equation $p(t) = \omega$ has only two real roots, i.e. $\tau \in (0, 1)$ and $\frac{1}{\tau} \in (1, \infty)$. Hence it suffices to show

$$p(\omega + \frac{2}{\omega^{n-1}}) < \omega < p(\omega + \frac{1}{\omega^{n-2}}),$$

then by Intermediate Value Theorem

$$\omega + \frac{2}{\omega^{n-1}} < \frac{1}{\tau} < \omega + \frac{1}{\omega^{n-2}}.$$

Take $\eta = \omega + \frac{2}{\omega^{n-1}}$ for short, then

$$\begin{aligned} p(\eta) < \omega &\iff \eta^{n+1} + 1 < \omega\eta^n + \omega\eta \\ &\iff (\eta - \omega)\eta^n < \omega\eta - 1 \\ &\iff \frac{2\eta^n}{\omega^{n-1}} < \omega(\omega + \frac{2}{\omega^{n-1}}) - 1 \\ &\iff 2(\frac{\eta}{\omega})^n < \omega + \frac{2}{\omega^{n-1}} - \frac{1}{\omega} \\ &\iff 2(1 + \frac{2}{\omega^n})^n < \omega - \frac{1}{\omega} + \frac{2}{\omega^{n-1}} \end{aligned} \tag{2.24}$$

Since ω^n/n increases with n and for $\omega > 2$, and $3^3/3 = 9 > 8$,

$$\omega^n > 8n \qquad \text{if } n,\, \omega \geq 3.$$

Also notice that the sequence $(1 + \frac{1}{k})^k$ is strictly increasing with limit e. Hence

$$(1 + \frac{1}{k})^k < e \qquad \text{for } k > 0.$$

The inequality (2.24) is always true since

$$2(1 + \frac{2}{\omega^n})^n < 2(1 + \frac{2}{8n})^n < 2\sqrt[4]{e} < 3 - \frac{1}{3} < \omega - \frac{1}{\omega} + \frac{2}{\omega^{n-1}}.$$

Similarly for the other inequality, substitute $\xi = \omega + \frac{1}{\omega^{n-2}}$, then

$$\begin{aligned} p(\xi) > \omega &\iff (\xi - \omega)\xi^n > \omega\xi - 1 \\ &\iff \frac{\xi^n}{\omega^{n-2}} > \omega(\omega + \omega^{2-n}) - 1 \\ &\iff (\frac{\xi}{\omega})^n > 1 + \omega^{1-n} - \omega^{-2}. \end{aligned}$$

The last inequality is always true since

$$(1 + \omega^{1-n})^n > 1 + n\omega^{1-n} + \cdots > 1 + n\omega^{1-n} > 1 + \omega^{1-n} - \omega^{-2}.$$

ii. Recall that q is defined by (2.14) and for $\omega > 1$ equation $q(t) = \omega$ has only two real roots, i.e. $\tau' \in (0,1)$ and $\frac{1}{\tau'} \in (1,\infty)$. Let $\xi' = \omega - \frac{1}{\omega^{n-2}}$, then

$$q(\xi') < \omega \iff (\xi')^{n+1} - 1 < \omega(\xi')^n - \omega\xi'$$

$$\begin{aligned} &\iff \omega\xi - 1 < (\omega - \xi')(\xi')^n \\ &\iff \omega^2 - \omega^{3-n} - 1 < \frac{(\xi')^n}{\omega^{n-2}} \\ &\iff 1 - \omega^{1-n} - \omega^{-2} < (\frac{\xi'}{\omega})^n. \end{aligned} \tag{2.25}$$

We need following inequalities, which can be proved by calculus or by induction,

$$(1-\delta)^n > 1 - n\delta \qquad \text{for } n > 1 \text{ and } 0 < \delta < 1,$$

$$\omega^{n-3} + 1 > n \qquad \text{if } n \geq 4 \text{ and } \omega > 3.$$

Indeed (2.25) holds since

$$(1-\omega^{1-n})^n > 1 - n\omega^{1-n} > 1 - (\omega^{n-3}+1)\omega^{1-n} = 1 - \omega^{1-n} - \omega^{-2}.$$

For the other inequality, consider $\eta' = \omega - \frac{2}{\omega^{n-1}}$, then

$$\begin{aligned} q(\eta') > \omega \quad &\iff \omega\eta' - 1 > (\omega - \eta')(\eta')^n \\ &\iff \omega(\omega - \frac{2}{\omega^{n-1}}) - 1 > \frac{2(\eta')^n}{\omega^{n-1}} \\ &\iff \omega - \frac{1}{\omega} - \frac{2}{\omega^{n-1}} > 2(\frac{\eta'}{\omega})^n. \end{aligned}$$

Obviously the last inequality is true since

$$\omega - \frac{1}{\omega} - \frac{2}{\omega^{n-1}} > 3 - \frac{1}{3} - \frac{2}{3^3} > 2 > 2(1 - \frac{2}{\omega^n})^n.$$

□

We remark that Lemma 2.2 (ii) fails when $n = 3$, since

$$\frac{1}{\tau'} = \omega - \frac{1}{\omega} - \frac{1}{\omega^3} - O(\frac{1}{\omega^5}) < \omega - \frac{1}{\omega^{n-2}}$$

by (2.21). Now the following theorem can be derived from Lemma 2.2.

Theorem 2.3 *Let λ_n and λ_{n-1} be the dominant eigenvalues of $J_n(\mathbf{w_1})$.*
Assume $\omega > 3$, then

i. *for $n \geq 2$,* $\omega + \frac{1}{\omega+\omega^{2-n}} + \frac{2}{\omega^{n-1}} < \lambda_n < \omega + \frac{1}{\omega+2\omega^{1-n}} + \frac{1}{\omega^{n-2}}$;

ii. *for $n \geq 4$,* $\omega + \frac{1}{\omega-2\omega^{1-n}} - \frac{1}{\omega^{n-2}} < \lambda_{n-1} < \omega + \frac{1}{\omega-\omega^{2-n}} - \frac{2}{\omega^{n-1}}$;

iii. *for $n \geq 3$,* $\frac{2}{\omega^{n-1}} < \frac{4}{\omega^{n-1}} - \frac{2}{\omega^n(1-\omega^{2-2n})} < \lambda_n - \lambda_{n-1} < \frac{2}{\omega^{n-2}} - \frac{4}{\omega^{n+1}(1-4\omega^{-2n})} < \frac{2}{\omega^{n-2}}$.

Proof.

i. Assume $n \geq 3$, then by Lemma 2.2 (i)

$$\frac{1}{\omega + \omega^{2-n}} < \tau < \frac{1}{\omega + 2\omega^{1-n}}$$

and

$$\omega + \frac{1}{\omega + \omega^{2-n}} + \frac{2}{\omega^{n-1}} < \tau + \frac{1}{\tau} < \omega + \frac{1}{\omega + 2\omega^{1-n}} + \frac{1}{\omega^{n-2}}.$$

The desired inequality follows from (2.15). It is trivial for the case $n = 2$ since

$$\omega + \frac{1}{\omega + 1} + \frac{2}{\omega} < \lambda_n = \omega + 1 < \omega + \frac{1}{\omega + 2\omega^{-1}} + 1.$$

ii. Similarly by Lemma 2.2 (ii)

$$\frac{1}{\omega - 2\omega^{1-n}} < \tau' < \frac{1}{\omega - \omega^{2-n}}$$

and

$$\omega + \frac{1}{\omega - 2\omega^{1-n}} - \frac{1}{\omega^{n-2}} < \lambda_{n-1} = \tau' + \frac{1}{\tau'} < \omega + \frac{1}{\omega - \omega^{2-n}} - \frac{2}{\omega^{n-1}}.$$

iii. According to (i) and (ii)

$$\begin{aligned} \lambda_n - \lambda_{n-1} &> \frac{4}{\omega^{n-1}} + \frac{1}{\omega + \omega^{2-n}} - \frac{1}{\omega - \omega^{2-n}} \\ &= \frac{4}{\omega^{n-1}} - \frac{2}{\omega^n(1 - \omega^{2-2n})} \\ &> \frac{4}{\omega^{n-1}} - \frac{2\omega}{\omega^n} = \frac{2}{\omega^{n-1}}, \end{aligned}$$

if $n \geq 4$, since

$$\frac{1}{1 - \omega^{2-2n}} < \frac{1}{1 - \frac{1}{2}} = 2 < \omega.$$

Similarly

$$\lambda_n - \lambda_{n-1} < \frac{2}{\omega^{n-2}} + \frac{1}{\omega + 2\omega^{1-n}} - \frac{1}{\omega - 2\omega^{1-n}} = \frac{2}{\omega^{n-2}} - \frac{4}{\omega^{n+1}(1 - 4\omega^{-2n})} < \frac{2}{\omega^{n-2}}.$$

The case $n = 3$ comes from straight computation. In view of (2.23), we want

$$\begin{aligned} & \frac{4}{\omega^2} - \frac{2}{\omega^3(1 - \omega^{-4})} < \frac{1}{2}(\sqrt{\omega^2 + 8} - \omega) < \frac{2}{\omega} - \frac{4}{\omega^4(1 - 4\omega^{-6})} \\ \iff\ & \omega + \frac{8}{\omega^2} - \frac{4}{\omega^3 - \omega^{-1}} < \sqrt{\omega^2 + 8} < \omega + \frac{4}{\omega} - \frac{8}{\omega^4 - 4\omega^{-2}} \\ \iff\ & \frac{64}{\omega^4} + \frac{16}{(\omega^3 - \omega^{-1})^2} + \frac{16}{\omega} - \frac{8\omega}{\omega^3 - \omega^{-1}} - \frac{64}{\omega^2(\omega^3 - \omega^{-1})} - 8 \\ & < 0 < \frac{16}{\omega^2} + \frac{64}{(\omega^4 - 4\omega^{-2})^2} - \frac{16\omega}{\omega^4 - 4\omega^{-2}} - \frac{64}{\omega(\omega^4 - 4\omega^{-2})}. \end{aligned} \tag{2.26}$$

The first inequality in (2.26) holds since

$$\frac{8}{\omega^4} + \frac{2}{(\omega^3 - \omega^{-1})^2} + \frac{2}{\omega} < \frac{8}{3^4} + \frac{2}{(3^3 - 1)^2} + \frac{2}{3} < 1,$$

and the second one holds since

$$\frac{\omega}{\omega^4 - 4\omega^{-2}} - \frac{4}{\omega(\omega^4 - 4\omega^{-2})} = \frac{1}{\omega^2}\left[\frac{1}{\omega - 4\omega^{-5}} + \frac{4}{\omega^3 - 4\omega^{-3}}\right] < \frac{1}{\omega^2}\left(\frac{1}{2} + \frac{4}{26}\right) < \frac{1}{\omega^2}.$$

□

2.4 Dual matrix $J_n(\mathbf{w_1}^*)$

The dual matrix

$$J_n(\mathbf{w_1}^*) = \text{tridiag}\begin{pmatrix} & 1 & & 1 & \cdots & 1 & & 1 & \\ 0 & & \omega & \cdot & \cdots & \cdot & \omega & & 0 \\ & 1 & & 1 & \cdots & 1 & & 1 & \end{pmatrix}$$

shares the same gap with $J_n(\mathbf{w_1})$. Therefore $J_n(\mathbf{w_1}^*)$ is also an extremal matrix. However all of its eigenvalues can be recovered from those of $J_n(\mathbf{w_1})$. Indeed by Theorem 1.4 (iii)

$$\lambda_i(J_n(\mathbf{w_1}^*)) = \omega - \lambda_{n-i}(J_n(\mathbf{w_1})) \qquad \text{for } i = 1, 2, \ldots, n. \tag{2.27}$$

In view of (2.19), (2.22) and (2.27), $J_n(\mathbf{w_1}^*)$ has

$$\lambda_1 = -\frac{1}{\omega} - \frac{(\omega - \frac{1}{\omega})^2}{\omega^n} + \frac{n-1}{\omega^{2n-3}} - \frac{3n-1}{\omega^{2n-1}} + \frac{3n+1}{\omega^{2n+1}} - \frac{n+1}{\omega^{2n+3}} - \frac{(n-1)(3n-2)}{2\omega^{3n-4}} + O\left(\frac{1}{\omega^{3n-2}}\right)$$

and

$$\lambda_2 = -\frac{1}{\omega} + \frac{(\omega - \frac{1}{\omega})^2}{\omega^n} + \frac{n-1}{\omega^{2n-3}} - \frac{3n-1}{\omega^{2n-1}} + \frac{3n+1}{\omega^{2n+1}} - \frac{n+1}{\omega^{2n+3}} + \frac{(n-1)(3n-2)}{2\omega^{3n-4}} + O\left(\frac{1}{\omega^{3n-2}}\right)$$

asymptotically. Similarly we have counter parts of Theorem 2.1 and 2.3.

Corollary 2.4 *Let λ_1 and λ_2 be two smallest eigenvalues of $J_n(\mathbf{w_1}^*)$, then*

i. for $n \geq 2$, $\quad \lambda_2 - \lambda_1 = \frac{2(\omega - \frac{1}{\omega})^2}{\omega^n} + \frac{(n-1)(3n-2)}{\omega^{3n-4}} + O(\frac{1}{\omega^{3n-2}}) \quad$ *as* $\omega \to \infty$;

ii. for $n \geq 2$ *and* $\omega > 3$, $\quad -\frac{1}{\omega + 2\omega^{1-n}} - \frac{1}{\omega^{n-2}} < \lambda_1 < -\frac{2}{\omega^{n-1}} - \frac{1}{\omega + \omega^{2-n}}$;

iii. for $n \geq 4$ *and* $\omega > 3$, $\quad -\frac{1}{\omega - \omega^{2-n}} + \frac{2}{\omega^{n-1}} < \lambda_2 < -\frac{1}{\omega - 2\omega^{1-n}} + \frac{1}{\omega^{n-2}}$;

iv. for $n \geq 3$ *and* $\omega > 3$,

$$\frac{2}{\omega^{n-1}} < \frac{4}{\omega^{n-1}} - \frac{2}{\omega^n(1 - \omega^{2-2n})} < \lambda_2 - \lambda_1 < \frac{2}{\omega^{n-2}} - \frac{4}{\omega^{n+1}(1 - 4\omega^{-2n})} < \frac{2}{\omega^{n-2}}.$$

Chapter 3

Ratios of Eigenvectors

Important to our minimization problem are the results on ratios of entries of eigenvectors, the subject of this chapter. We consider unreduced symmetric tridiagonal matrices

$$T_n(\mathbf{a}) = \text{tridiag}\begin{pmatrix} & \beta_1 & \cdots & \beta_{n-1} & \\ a(1) & \cdot & \cdots & \cdots & a(n) \\ & \beta_1 & \cdots & \beta_{n-1} & \end{pmatrix}$$

with the diagonal $\mathbf{a} = (a(1), a(2), \ldots, a(n))$, and all the β_i's positive.

Assume $T(\mathbf{a})$ has eigenvalues $\lambda_1 < \lambda_2 < \cdots < \lambda_n$. Let $\mathbf{v_i} = (v_i(1), v_i(2), \ldots, v_i(n))$ be an eigenvector corresponding to λ_i, and $\mathbf{s_i} = (s_i(1), s_i(2), \ldots, s_i(n))$ be the normalized eigenvector. Notice that $v_1(i)$, $v_n(i)$, $v_i(1)$ and $v_i(n)$ are nonzero for all i's [9, 7-9-5]. Hence we assume all $v_i(1)$'s are positive in the whole chapter, though the theorems apply to general $v_i(1)$'s.

For $i = 1, 2, \ldots, n$, we can write $T(\mathbf{a})\mathbf{v_i} = \lambda_i \mathbf{v_i}$ as a system of linear equations

$$\beta_{k-1} v_i(k-1) + (a(k) - \lambda_i) v_i(k) + \beta_k v_i(k+1) = 0, \tag{3.1}$$

where $v_i(0) = v_i(n+1) = 0$. From (3.1) there cannot be two consecutive zeros in an eigenvector. If $v_i(k) \neq 0$, then

$$\beta_{k-1} \frac{v_i(k-1)}{v_i(k)} + \beta_k \frac{v_i(k+1)}{v_i(k)} = \lambda_i - a(k) \tag{3.2}$$

This ratio equation is the key tool that leads to all the theorems.

3.1 Ratio of $\mathbf{v_{n-1}}$ and $\mathbf{v_n}$

(3.2) governs the ratios of consecutive entries of an eigenvector. It's not surprising that our first lemma uncovers the relation between the ratios of adjacent entries of $\mathbf{v_i}$ and those of $\mathbf{v_j}$.

Lemma 3.1 *Assume $j > i$ and $v_i(k)v_j(k) > 0$ for $k = 1, 2, \cdots, \ell$, then*

$$\frac{v_j(k)}{v_j(k-1)} > \frac{v_i(k)}{v_i(k-1)}. \tag{3.3}$$

for $k = 2, 3, \ldots, \ell + 1$.

Proof. Recall that $\lambda_j > \lambda_i$. For $k = 2$,

$$\frac{v_j(2)}{v_j(1)} = \frac{\lambda_j - a(1)}{\beta_1} > \frac{\lambda_i - a(1)}{\beta_1} = \frac{v_i(2)}{v_i(1)}$$

by (3.2). Suppose (3.3) holds for some $k \leq \ell$, then

$$-\frac{v_j(k-1)}{v_j(k)} > -\frac{v_i(k-1)}{v_i(k)}, \tag{3.4}$$

since both ratios in (3.3) are positive by assumption. In view of (3.2),

$$\beta_{k-1}\frac{v_j(k-1)}{v_j(k)} + \beta_k\frac{v_j(k+1)}{v_j(k)} = \lambda_j - a(k) > \lambda_i - a(k) = \beta_{k-1}\frac{v_i(k-1)}{v_i(k)} + \beta_k\frac{v_i(k+1)}{v_i(k)}. \tag{3.5}$$

Multiply (3.4) by β_{k-1} and add it to (3.5), then

$$\frac{v_j(k+1)}{v_j(k)} > \frac{v_i(k+1)}{v_i(k)}$$

as desired. By induction (3.3) holds whenever $v_i(k)v_j(k) > 0$. □

If we have $v_i(k)v_j(k) < 0$ in Lemma 3.1, then the inequality (3.3) reverses. Also it is possible to replace $k = 1, 2, \cdots, \ell$ by $k = \ell', \ell' + 1, \ldots, n$ in Lemma 3.1. Here comes our main theorem, which states that the element-by-element ratio of $\mathbf{v_{n-1}}$ and $\mathbf{v_n}$ is strictly monotonic.

Theorem 3.2 *Under the normalization $v_{n-1}(1)v_n(1) > 0$, then $\frac{v_{n-1}(k)}{v_n(k)}$ is a strictly decreasing sequence in k.*

Proof. Without loss of generality, we may assume $v_n(1)$ and $v_{n-1}(1)$ are positive. Then $v_n(k) > 0$ for all k's since $\mathbf{v_n}$ has no sign change. Because $\mathbf{v_{n-1}}$ has exactly one sign reversal, there is an integer $\ell \le n-1$ such that

$$v_{n-1}(1) > 0, \ldots, v_{n-1}(\ell-1) > 0, v_{n-1}(\ell) \ge 0, v_{n-1}(\ell+1) < 0, \ldots, v_{n-1}(n) < 0.$$

Take $i = n-1$ and $j = n$ in Lemma 3.1 to find

$$\frac{v_n(k)}{v_n(k-1)} > \frac{v_{n-1}(k)}{v_{n-1}(k-1)},$$

$$\text{or} \qquad \frac{v_{n-1}(k-1)}{v_n(k-1)} > \frac{v_{n-1}(k)}{v_n(k)}$$

for $k = 2, 3, \ldots, \ell$. Hence

$$\frac{v_{n-1}(1)}{v_n(1)} > \frac{v_{n-1}(2)}{v_n(2)} > \cdots > \frac{v_{n-1}(\ell)}{v_n(\ell)} \ge 0 > \frac{v_{n-1}(\ell+1)}{v_n(\ell+1)}. \tag{3.6}$$

The rest of inequalities can be proved by the symmetry of the eigenvectors. Recall $\tilde{I}$ from Theorem 1.4, then $\tilde{T} := \tilde{I}T(a)\tilde{I}$ just reverses the diagonals. By Theorem 1.4, $\tilde{T}$ has the same eigenvalues $\{\lambda_i\}$, but eigenvectors $\{\mathbf{v_i}^R\}$ in reverse order, i.e.

$$v_i^R(k) = v_i(n+1-k) \qquad \text{for } i, k = 1, 2, \ldots, n. \tag{3.7}$$

Notice that $v_n^R(k) > 0$ for all k, and $v_{n-1}^R(k) < 0$ for $k = 1, 2, \ldots, n-\ell$. Apply (3.6) to eigenvectors $\mathbf{v_n^R}$ and $-\mathbf{v_{n-1}^R}$, then

$$-\frac{v_{n-1}^R(1)}{v_n^R(1)} > -\frac{v_{n-1}^R(2)}{v_n^R(2)} > \cdots > -\frac{v_{n-1}^R(n-\ell)}{v_n^R(n-\ell)} > 0 \ge -\frac{v_{n-1}^R(n-\ell+1)}{v_n^R(n-\ell+1)}.$$

Therefore by (3.7)

$$\frac{v_{n-1}(n)}{v_n(n)} < \frac{v_{n-1}(n-1)}{v_n(n-1)} < \cdots < \frac{v_{n-1}(\ell+1)}{v_n(\ell+1)} < 0 \le \frac{v_{n-1}(\ell)}{v_n(\ell)},$$

which concludes the proof. □

We remark that $\frac{v_{n-1}(k)}{v_n(k)}$ is strictly increasing in k when $v_{n-1}(1)v_n(1) < 0$. Needless to say, the normalized eigenvectors $\mathbf{s_i}$'s obey Lemma 3.1 and Theorem 3.2. However we obtain more by using the normalization of $\mathbf{s_i}$'s.

Corollary 3.3 *For $n \ge 3$, either $|s_{n-1}(1)| > |s_n(1)|$ or $|s_{n-1}(n)| > |s_n(n)|$.*

Proof. Suppose $s_n(1)$, $s_{n-1}(1) > 0$ and the assertion is false, i.e.

$$s_n(1) \geq s_{n-1}(1) \qquad \text{and} \qquad -s_{n-1}(n) \leq s_n(n).$$

Thus by Theorem 3.2

$$1 \geq \frac{s_{n-1}(1)}{s_n(1)} > \frac{s_{n-1}(2)}{s_n(2)} > \cdots > \frac{s_{n-1}(n)}{s_n(n)} \geq -1.$$

Hence for all k's

$$1 \geq \left|\frac{s_{n-1}(k)}{s_n(k)}\right| \qquad \text{or} \qquad |s_n(k)| \geq |s_{n-1}(k)|$$

with at least one strict inequality. Then we have a contradiction

$$1 = \sum_{k=1}^{n} s_n(k)^2 > \sum_{k=1}^{n} s_{n-1}(k)^2 = 1.$$

□

By Corollary 3.3 and $||\mathbf{s_n}||_2^2 = ||\mathbf{s_{n-1}}||_2^2 = 1$, there exists an integer k such that $|s_n(k)| > |s_{n-1}(k)|$. More precisely we have

Corollary 3.4 *Suppose $n \geq 3$ and $s_{n-1}(\ell)s_{n-1}(\ell+1) \leq 0$ for some integer ℓ, then either $|s_n(\ell)| > |s_{n-1}(\ell)|$ or $|s_n(\ell+1)| > |s_{n-1}(\ell+1)|$.*

Proof. Again assume $s_n(1)$, $s_{n-1}(1) > 0$, $s_{n-1}(\ell) \geq s_n(\ell)$ and $s_n(\ell+1) \leq -s_{n-1}(\ell+1)$. Then by Theorem 3.2

$$\frac{s_{n-1}(1)}{s_n(1)} > \ldots > \frac{s_{n-1}(\ell)}{s_n(\ell)} \geq 1 > -1 \geq \frac{s_{n-1}(\ell+1)}{s_n(\ell+1)} > \cdots > \frac{s_{n-1}(n)}{s_n(n)},$$

$$\text{i.e.} \quad |s_{n-1}(k)| \geq |s_n(k)| \qquad \text{for } k = 1, 2, \ldots, n$$

with at least one strict inequality. Therefore

$$1 = \sum_{k=1}^{n} s_{n-1}(k)^2 > \sum_{k=1}^{n} s_n(k)^2 = 1.$$

which is a contradiction. Hence $s_{n-1}(k) \geq s_n(k)$ for $k = \ell$ or $\ell + 1$. □

We remark that Corollary 3.3 and Corollary 3.4 may fail for the case $n = 2$. For example $J_2(0)$ has eigenvalues ± 1 and corresponding eigenvectors $(\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}})$ and $(\frac{1}{\sqrt{2}}, \frac{-1}{\sqrt{2}})$. This is a counterexample.

To illustrate Theorem 3.2 and Corollary 3.3-4, consider $J_{10}((2, 0, \ldots, 0, 2))$, which has ratio vector $s_9(k)/s_{10}(k)$

$$(1.0098, 1.0010, 0.9579, 0.7953, 0.3416, -0.3416, -0.7953, -0.9579, -1.0010, -1.0098),$$

Figure 3.1 gives another example.

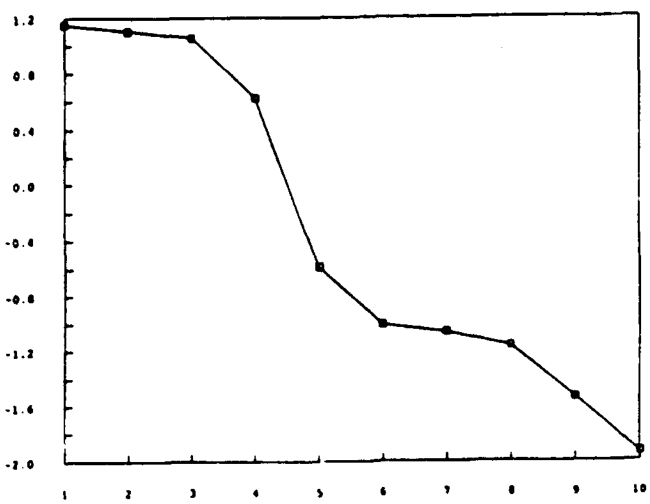

Figure 3.1: $\frac{s_9(k)}{s_{10}(k)}$ of $J_10((0,0,3,0,0,3,0,0,0,3))$.

3.2 Sign Pattern of ∇g_{n-1}

Recall that the separation $g_{n-1}(T(\mathbf{a})) := \lambda_n(T(\mathbf{a})) - \lambda_{n-1}(T(\mathbf{a}))$ is a real valued multi-variable function. Its gradient is given by Lemma 1.6

$$\nabla g_{n-1}(T(\mathbf{a})) = (s_n(1)^2 - s_{n-1}(1)^2, s_n(2)^2 - s_{n-1}(2)^2, \ldots, s_n(n)^2 - s_{n-1}(n)^2). \qquad (3.8)$$

As a consequence of Corollary 3.3 or 3.4, $\nabla g_{n-1} \neq \mathbf{0}$ for $n \geq 3$ and all $\mathbf{a}$'s. This certainly is not true for $n = 2$, $J_2(\mathbf{0})$ in the previous section is an example.

Assume $n \geq 3$ and $s_n(1)$, $s_{n-1}(1) > 0$ in the sequel. According to Corollary 3.3, there are three cases

I. $\quad s_{n-1}(1) > s_n(1) \quad$ and $\quad -s_{n-1}(n) \leq s_n(n)$;

II. $\quad s_{n-1}(1) \leq s_n(1) \quad$ and $\quad -s_{n-1}(n) > s_n(n)$;

III. $\quad s_{n-1}(1) > s_n(1) \quad$ and $\quad -s_{n-1}(n) > s_n(n)$.

Combined with Theorem 3.2, each case gives

I. $\quad \frac{s_{n-1}(1)}{s_n(1)} > \ldots > \frac{s_{n-1}(i)}{s_n(i)} > 1 \geq \frac{s_{n-1}(i+1)}{s_n(i+1)} > \cdots > \frac{s_{n-1}(n)}{s_n(n)} \geq -1$;

II. $\quad 1 \geq \frac{s_{n-1}(1)}{s_n(1)} > \ldots > \frac{s_{n-1}(j-1)}{s_n(j-1)} \geq -1 > \frac{s_{n-1}(j)}{s_n(j)} > \cdots > \frac{s_{n-1}(n)}{s_n(n)}$;

III. $\quad \ldots > \frac{s_{n-1}(i)}{s_n(i)} > 1 \geq \frac{s_{n-1}(i+1)}{s_n(i+1)} > \cdots > \frac{s_{n-1}(j-1)}{s_n(j-1)} \geq -1 > \frac{s_{n-1}(j)}{s_n(j)} > \cdots$

for some integers i and j. Therefore the gradient (3.8) has corresponding sign patterns

I. $(-,-,\ldots,\underbrace{-}_{\text{i-th}},+0,+,\ldots,+,+0);$

II. $(+0,+,\ldots,+,+0,\underbrace{-}_{\text{j-th}},-,\ldots,-);$

III. $(-,\ldots,\underbrace{-}_{\text{i-th}},+0,+,\ldots,+,+0,\underbrace{-}_{\text{j-th}},\ldots,-).$

Here "+0" means the entry can be positive or zero.

Recall from the end of last section, the ratio vector $s_9(k)/s_{10}(k)$ of $J_{10}((2,0,\ldots,0,2))$ is skew symmetric. This is true for all centrosymmetric tridiagonal $T(\mathbf{a})$ since its eigenvectors are either symmetric or skew symmetric by Corollary 1.10 (i). Therefore we can replace "or" by "and" in Corollary 3.3 and 3.4.

Corollary 3.5 *Assume $T(\mathbf{a})$ is centrosymmetric and $n \geq 3$, then*

i. $|s_{n-1}(1)| > |s_n(1)|$ *and* $|s_{n-1}(n)| > |s_n(n)|$;

ii. $|s_n(k)| > |s_{n-1}(k)|$ *for* $k = [\frac{n}{2}],\ldots,[\frac{n+3}{2}]$.

Only case (III) above is possible for centrosymmetric T. The gradient ∇g_{n-1} is also symmetric about the center and has the sign pattern

$$\nabla g_{n-1} = (-,\ldots,\underbrace{-}_{i\text{-th}},+0,+,\ldots,+,+0,\underbrace{-}_{(n+1-i)\text{-th}},\ldots,-). \tag{3.9}$$

Now we are ready to prove Ashbaugh and Benguria's Comparison Theorem [1, Theorem 5.1]. They only prove it for $J(\mathbf{a})$, but in fact it is true for all centrosymmetric $T(\mathbf{a})$.

Definition 4 *A vector $\mathbf{u} = (u(1),u(2),\ldots,u(n))$ is symmetric increasing (from the center) if*

$$u(1) = u(n) \geq u(2) = u(n-1) \geq \cdots \geq u([\frac{n+1}{2}]) = u([\frac{n}{2}]+1).$$

Theorem 3.6 (Ashbaugh and Benguria) *Assume $T(\mathbf{a})$ is centrosymmetric and $\mathbf{u}$ is symmetric increasing, then*

$$g_{n-1}(T(\mathbf{a}+\mathbf{u})) \leq g_{n-1}(T(\mathbf{a})). \tag{3.10}$$

Equality holds if and only if all the entries of $\mathbf{u}$ are the same.

Proof. The case $n = 2$ is nothing but a shift (or translation) of T, so equality always holds. Assume $n \geq 3$. By the Mean Value Theorem, there exits $\eta \in (0, 1)$ such that

$$g_{n-1}(T(\mathbf{a} + \mathbf{u})) - g_{n-1}(T(\mathbf{a})) = \nabla g_{n-1}(T(\mathbf{a} + \eta\mathbf{u})) \cdot \mathbf{u}. \tag{3.11}$$

By assumption $\mathbf{a}$ and $\mathbf{u}$ are centrally symmetric, then so is $\mathbf{a} + \eta\mathbf{u}$. Thus $T(\mathbf{a} + \eta\mathbf{u}))$ is also centrosymmetric and we can assume $\nabla g_{n-1}(T(\mathbf{a} + \eta\mathbf{u}))$ has sign pattern (3.9) for some i.

Now we translate $\mathbf{u}$ to

$$\mathbf{u}' := \mathbf{u} - u(i+1)\mathbf{e},$$

where $\mathbf{e} = (1, 1, \ldots, 1)$. Since $u'(k) = u(k) - u(i+1)$ for $k = 1, 2, \ldots, n$, $\mathbf{u}$' has the sign pattern

$$\mathbf{u}' = (+0, \ldots, \underbrace{+0}_{i\text{-th}}, 0, -0, \ldots, -0, 0, \underbrace{+0}_{(n+1-i)\text{-th}}, \ldots, +0). \tag{3.12}$$

by the symmetric increase of $\mathbf{u}$. Again "+0" means the entry ≥ 0 and "-0" means ≤ 0. Match the patterns of (3.9) and (3.12) to get

$$\nabla g_{n-1}(T(\mathbf{a} + \eta\mathbf{u})) \cdot \mathbf{u}' \leq 0, \tag{3.13}$$

Hence

$$\nabla g_{n-1}(T(\mathbf{a} + \eta\mathbf{u})) \cdot \mathbf{u} = \nabla g_{n-1}(T(\mathbf{a} + \eta\mathbf{u})) \cdot \mathbf{u}' + u(i+1)\nabla g_{n-1}(T(\mathbf{a} + \eta\mathbf{u})) \cdot \mathbf{e} \leq 0$$

since the last term vanishes by Corollary 1.7 (ii). Then (3.10) follows by (3.11).

If $\mathbf{u} = \sigma\mathbf{e}$ for some scalar σ, then (3.10) becomes equality by Corollary 1.5 (i). For another direction, suppose we have equality in (3.10), then so is (3.13)

$$\sum_{k=1}^{n} \xi_k u'(k) = 0 \tag{3.14}$$

where $\nabla g_{n-1}(T(\mathbf{a} + \eta\mathbf{u})) = (\xi_1, \xi_2, \ldots, \xi_n)$. Since (3.14) has no positive term, $\xi_k u'(k)$ vanishes for all k's. Notice that $\xi_1 < 0$ and $\xi_{[\frac{n+1}{2}]} > 0$ by (3.8) and Corollary 3.5. Therefore

$$u'(1) = u'([\frac{n+1}{2}]) = 0 \qquad \text{or} \qquad u(1) = u(i+1) = u([\frac{n+1}{2}]).$$

By symmetric increase of $\mathbf{u}$, all the entries of $\mathbf{u}$ are equal. $\square$

3.3 Unbalanced Diagonals

In this section we consider $T(\mathbf{a})$ with unbalanced diagonals. We assume the right side is heavier than the left for the main diagonal and two subdiagonals, though the reverse case can be treated similarly. The ratios of two consecutive entries of an eigenvector obey a certain rule, which will be explored here. We start with the following lemma.

Lemma 3.7 *Let* $\mathbf{v_i}$ *be the i-th eigenvector of* $T(\mathbf{a})$. *Assume*

$$\begin{cases} v_i(1), v_i(2), \ldots, v_i(\ell) \text{ have the same signs,} \\ \text{and so do } v_i(n+1-\ell), v_i(n+2-\ell), \ldots, v_i(n); \end{cases} \tag{3.15}$$

$$a(k) \le a(n+1-k) \qquad \text{for } k = 1, 2, \ldots, \ell; \tag{3.16}$$

$$\beta_k \le \beta_{n-k} \qquad \text{for } k = 1, 2, \ldots, \ell; \tag{3.17}$$

for some $\ell \le [\frac{n}{2}]$, *and* j *is the first index* k *that gives strict inequality in (3.16) or (3.17). Then*

i. $\frac{v_i(k+1)}{v_i(k)} = \frac{v_i(n-k)}{v_i(n+1-k)}$ *for* $k = 1, 2, \ldots, \min\{j-1, \ell\}$;

ii. $\frac{v_i(k+1)}{v_i(k)} > \frac{v_i(n-k)}{v_i(n+1-k)}$ *for* $k = j, j+1, \ldots, \ell$.

We give two remarks before the proof. In the case $j = 1$, (i) is not necessary in Lemma 3.7. If equality holds everywhere in (3.16) and (3.17), then we can take $j = \ell + 1$ and part (ii) is redundant.

Proof. Since neither $v_i(1)$ nor $v_i(n)$ vanishes,

$$v_i(k) \neq 0 \qquad \text{for all } k = 1, \ldots, \ell \text{ and } n+1-\ell, \ldots, n$$

by (3.15). Hence it is legitimate to take ratios

$$\frac{v_i(k+1)}{v_i(k)} \qquad \text{and} \qquad \frac{v_i(n-k)}{v_i(n+1-k)} \tag{3.18}$$

for $k = 1, 2, \ldots, \ell$. Moreover both ratios in (3.18) are positive for $k = 1, 2, \ldots, \ell - 1$ by (3.15).

i. Suppose $j > 1$, then by assumption

$$a(k) = a(n+1-k) \quad \text{and} \quad \beta_k = \beta_{n-k} \qquad \text{for } k = 1, 2, \ldots, j-1. \tag{3.19}$$

Our induction argument begins with

$$\frac{v_i(2)}{v_i(1)} = \frac{\lambda_i - a(1)}{\beta_1} = \frac{\lambda_i - a(i)}{\beta_{n-1}} = \frac{v_i(n-1)}{v_i(n)}$$

by (3.2) and (3.19). Now assume

$$\frac{v_i(k)}{v_i(k-1)} = \frac{v_i(n-k+1)}{v_i(n-k+2)}$$

for some $k < j$, then by (3.19)

$$\beta_{k-1}\frac{v_i(k-1)}{v_i(k)} = \beta_{n+1-k}\frac{v_i(n-k+2)}{v_i(n-k+1)} \tag{3.20}$$

Use (3.2) and (3.19) again to get

$$\begin{aligned}
&\beta_{k-1}\frac{v_i(k-1)}{v_i(k)} + \beta_k\frac{v_i(k+1)}{v_i(k)} = \lambda_i - a(k) \\
= \quad &\lambda_i - a(n+1-k) = \beta_{n-k}\frac{v_i(n-k)}{v_i(n+1-k)} + \beta_{n+1-k}\frac{v_i(n+2-k)}{v_i(n+1-k)}.
\end{aligned} \tag{3.21}$$

Subtracting (3.20) from (3.21), we have

$$\frac{v_i(k+1)}{v_i(k)} = \frac{v_i(n-k)}{v_i(n-k+1)}$$

by (3.19). Part (i) follows by induction until $k = j$ or there is a sign change.

ii. Suppose $j \leq \ell$. From (i)

$$\frac{v_i(j)}{v_i(j-1)} = \frac{v_i(n+1-j)}{v_i(n+2-j)},$$

$$\beta_{j-1}\frac{v_i(j-1)}{v_i(j)} = \beta_{n+1-j}\frac{v_i(n+2-j)}{v_i(n+1-j)}. \tag{3.22}$$

According to (3.2) and (3.16)

$$\begin{aligned}
&\beta_{j-1}\frac{v_i(j-1)}{v_i(j)} + \beta_j\frac{v_i(j+1)}{v_i(j)} = \lambda_i - a(j) \\
\geq \quad &\lambda_i - a(n+1-j) = \beta_{n-j}\frac{v_i(n-j)}{v_i(n+1-j)} + \beta_{n+1-j}\frac{v_i(n+2-j)}{v_i(n+1-j)}.
\end{aligned} \tag{3.23}$$

Subtract (3.22) from (3.23), then

$$\beta_j\frac{v_i(j+1)}{v_i(j)} \geq \beta_{n-j}\frac{v_i(n-j)}{v_i(n+1-j)}. \tag{3.24}$$

By (3.17)

$$\frac{1}{\beta_j} \geq \frac{1}{\beta_{n-j}}. \tag{3.25}$$

Since

$$a(j) < a(n+1-j) \qquad \text{or} \qquad \beta_j < \beta_{n-j},$$

inequalities (3.23) and (3.24) are strict, or (3.25) is strict. Multiplying (3.24) and (3.25), we have

$$\frac{v_i(j+1)}{v_i(j)} > \frac{v_i(n-j)}{v_i(n+1-j)}.$$

Assume

$$\frac{v_i(k)}{v_i(k-1)} > \frac{v_i(n+1-k)}{v_i(n+2-k)}$$

for some $k < \ell$, then by (3.17)

$$-\beta_{k-1}\frac{v_i(k-1)}{v_i(k)} > -\beta_{n+1-k}\frac{v_i(n+2-k)}{v_i(n+1-k)} \tag{3.26}$$

Similarly by (3.2) and (3.16)

$$\begin{aligned}\beta_{k-1}\frac{v_i(k-1)}{v_i(k)} + \beta_k\frac{v_i(k+1)}{v_i(k)} &= \lambda_i - a(k)\\ = \quad \lambda_i - a(n+1-k) &\geq \beta_{n-k}\frac{v_i(n-k)}{v_i(n+1-k)} + \beta_{n+1-k}\frac{v_i(n+2-k)}{v_i(n+1-k)}.\end{aligned} \tag{3.27}$$

Add both (3.26) and (3.27), then multiply it with $\frac{1}{\beta_k} \geq \frac{1}{\beta_{n-k}}$ to get

$$\frac{v_i(k+1)}{v_i(k)} > \frac{v_i(n-k)}{v_i(n-k+1)}.$$

Below we consider

$$a(k) \leq a(n+1-k) \qquad \text{for } k = 1, 2, \ldots, [\frac{n}{2}], \tag{3.28}$$

$$\beta_k \leq \beta_{n-k} \qquad \text{for } k = 1, 2, \ldots, [\frac{n}{2}], \tag{3.29}$$

and apply Lemma 3.7 to $\mathbf{v_n}$ and $\mathbf{v_{n-1}}$. If at least one of the inequalities in (3.28) or (3.29) is strict, then positive $\mathbf{v_n}$ is heavier in the right side and the broken line graph of $\mathbf{v_{n-1}}$ crosses zero after the midpoint $\frac{n+1}{2}$.

Theorem 3.8 *Assume (3.28) and (3.29) hold, and j is the first k that gives strict inequality in (3.28) or (3.29). Then*

i. $\frac{v_n(k+1)}{v_n(k)} = \frac{v_n(n-k)}{v_n(n-k+1)}$ *for* $k = 1, 2, \ldots, j-1$;

ii. $\frac{v_n(k+1)}{v_n(k)} > \frac{v_n(n-k)}{v_n(n-k+1)}$ *for* $k = j, j+1, \ldots, [\frac{n}{2}]$;

iii. *if* $\mathbf{v_n}$ *is positive, then for* $k = 1, 2, \ldots, [\frac{n}{2}]$

$$v_n(k) < v_n(n+1-k). \tag{3.30}$$

Proof. Since $\mathbf{v_n}$ has no sign change, (3.15) is true for $\ell = [\frac{n}{2}]$. Now (i) and (ii) are exactly Lemma 3.7.

Consider (iii). From (ii) with $k = [\frac{n}{2}]$

$$\frac{v_n([\frac{n}{2}]+1)}{v_n([\frac{n}{2}])} > \frac{v_n(n-[\frac{n}{2}])}{v_n(n+1-[\frac{n}{2}])}.$$

Thus for odd n

$$\frac{v_n(\frac{n+1}{2})}{v_n(\frac{n-1}{2})} > \frac{v_n(\frac{n+1}{2})}{v_n(\frac{n+3}{2})} \quad \Rightarrow \quad v_n(\frac{n-1}{2}) < v_n(\frac{n+3}{2}),$$

and for even n

$$\frac{v_n(\frac{n}{2}+1)}{v_n(\frac{n}{2})} > \frac{v_n(\frac{n}{2})}{v_n(\frac{n}{2}+1)} \quad \Rightarrow \quad v_n(\frac{n}{2}) < v_n(\frac{n}{2}+1).$$

Hence (3.30) holds for $k = [\frac{n}{2}]$. Now we can prove this part by induction backward on k. Assume

$$v_n(k+1) < v_n(n-k) \tag{3.31}$$

for some $k > 1$. In view of (i-ii), we have

$$\frac{v_n(k)}{v_n(k+1)} \leq \frac{v_n(n-k+1)}{v_n(n-k)}. \tag{3.32}$$

Multiply (3.31) and (3.32), then (3.30) follows. □

In Theorem 3.8 we assumed at least one strict inequality in (3.28) or (3.29). Suppose they are all equalities, then Theorem 3.8 (i) holds for all $k = 1, 2, \ldots, [\frac{n}{2}]$ and (ii) is redundant. As in the proof of Theorem 3.8 (iii), we can show

$$v_n(k) = v_n(n+1-k) \qquad \text{for } k = 1, 2, \ldots, [\frac{n}{2}].$$

This gives the symmetry of $\mathbf{v_n}$ for centrosymmetric T, which is not new of course.

The next theorem considers $\mathbf{v_{n-1}}$. Notice that Lemma 3.7 is valid until it encounters the sign change of $\mathbf{v_{n-1}}$. The broken line graph of vector $\mathbf{v}$ is a piecewise linear curve that goes through all the nodes $(k, v(k))$.

Theorem 3.9 *Assume (3.28) and (3.29) with at least one strict inequality. Then*

i. *the zero γ of the broken line graph of $\mathbf{v_{n-1}}$ satisfies $\gamma > \frac{n+1}{2}$;*

ii. *if $v_{n-1}(1)$ is positive, then*

$$v_{n-1}(\tfrac{n+1}{2}) > 0 \textit{ for odd } n, \quad \textit{and } v_{n-1}(\tfrac{n}{2}) + v_{n-1}(\tfrac{n}{2}+1) > 0 \textit{ for even } n;$$

iii. $\frac{v_{n-1}(k+1)}{v_{n-1}(k)} \geq \frac{v_{n-1}(n-k)}{v_{n-1}(n-k+1)}$ *for $k = 1, 2, \ldots, n - [\gamma]$.*

Proof. Without loss of generality, we can assume $v_{n-1}(1) > 0$.

Suppose $\gamma \leq \frac{n}{2}$. Define

$$\ell := \begin{cases} \gamma - 1, & \text{if } \gamma \text{ is an integer;} \\ [\gamma], & \text{otherwise.} \end{cases}$$

Then

$$v_{n-1}(1) > 0, \ldots, v_{n-1}(\ell) > 0, v_{n-1}(\ell+1) \leq 0, v_{n-1}(\ell+2) < 0, \ldots, v_{n-1}(n) < 0.$$

Hence by Lemma 3.7

$$0 \geq \frac{v_{n-1}(\ell+1)}{v_{n-1}(\ell)} \geq \frac{v_{n-1}(n-\ell)}{v_{n-1}(n-\ell+1)} > 0,$$

which is impossible.

Suppose $\frac{n}{2} < \gamma \leq \frac{n+1}{2}$. When n is odd, we have

$$v_{n-1}(\frac{n-1}{2}) > 0, v_{n-1}(\frac{n+1}{2}) \leq 0, \text{ and } v_{n-1}(\frac{n+3}{2}) < 0.$$

Since there is at least one strict inequality in (3.28) or (3.29), by Lemma 3.7

$$0 \geq \frac{v_{n-1}(\frac{n+1}{2})}{v_{n-1}(\frac{n-1}{2})} > \frac{v_{n-1}(\frac{n+1}{2})}{v_{n-1}(\frac{n+3}{2})} \geq 0.$$

which is a contradiction. When n is even, we have

$$v_{n-1}(\frac{n}{2}) > 0, v_{n-1}(\frac{n}{2}+1) < 0, \text{ and } v_{n-1}(\frac{n}{2}) + v_{n-1}(\frac{n}{2}+1) \leq 0.$$

Again we have a contradiction by Lemma 3.7

$$-1 \geq \frac{v_{n-1}(\frac{n}{2}+1)}{v_{n-1}(\frac{n}{2})} > \frac{v_{n-1}(\frac{n}{2})}{v_{n-1}(\frac{n}{2}+1)} \geq -1.$$

Therefore γ must be larger than $\frac{n+1}{2}$. Since the broken line graph of $\mathbf{v_{n-1}}$ is positive at the midpoint $\frac{n+1}{2}$, (ii) follows. Part (iii) is exactly Lemma 3.7. □

Consider $J_{10}((2,2,0,0,0,0,0,0,2.1,2))$ as an example. Its eigenvectors

$$s_{10} = (0.0089, 0.0111, 0.0049, 0.0049, 0.0110, 0.0308, 0.0891, 0.2584, 0.7498, 0.6014),$$

$$s_9 = (0.6177, 0.7359, 0.2592, 0.0912, 0.0320, 0.0108, 0.0024, -0.0031, -0.0123, -0.0103)$$

illustrate well Theorem 3.8 and Theorem 3.9. Notice that $j = 2$ and $7 < \gamma < 8$.

3.4 Convexity

In this section we consider $T(\mathbf{a})$ with partially symmetric diagonals. We have following convexity property for the entries of an eigenvector.

Theorem 3.10 *Assume*

$$a(k) = a(n+1-k) \quad \text{and} \quad \beta_k = \beta_{n-k} > 0 \quad \text{for } k = j+1, j+2, \ldots, [\frac{n+1}{2}], \tag{3.33}$$

$$a(k) + 2\beta_k \leq \lambda_i \qquad \text{for } k = j+1, j+2, \ldots, [\frac{n+1}{2}], \tag{3.34}$$

for some $i \leq n$ *and* $j \leq [\frac{n+1}{2}]$. *Under the normalization*

$$\begin{cases} v_i(\frac{n+1}{2}) \geq 0, & \text{when } n \text{ is odd;} \\ v_i(\frac{n}{2}) + v_i(\frac{n}{2}+1) \geq 0, & \text{when } n \text{ is even;} \end{cases} \tag{3.35}$$

we have

$$\begin{aligned} \beta_j[v_i(j) + v_i(n+1-j)] &\geq \beta_{j+1}[v_i(j+1) + v_i(n-j)] \quad \geq \cdots \\ &\geq \beta_{[\frac{n+1}{2}]}[v_i([\frac{n+1}{2}]) + v_i([\frac{n}{2}]+1)] \;\geq 0. \end{aligned} \tag{3.36}$$

Proof. First assume n is odd, then $[\frac{n+1}{2}] = \frac{n+1}{2} = [\frac{n}{2}] + 1$. By (3.1), (3.33), (3.34) and (3.35)

$$\begin{aligned} & \beta_{\frac{n-1}{2}}[v_i(\frac{n-1}{2}) + v_i(\frac{n+3}{2})] = \beta_{\frac{n-1}{2}} v_i(\frac{n-1}{2}) + \beta_{\frac{n+1}{2}} v_i(\frac{n+3}{2}) \\ = \;& (\lambda_i - a(\frac{n+1}{2}))v_i(\frac{n+1}{2}) \geq 2\beta_{\frac{n-1}{2}} v_i(\frac{n+1}{2}) = \beta_{[\frac{n+1}{2}]}[v_i([\frac{n+1}{2}]) + v_i([\frac{n}{2}]+1)] \geq 0. \end{aligned}$$

The counter part of even n can be proved by a similar fashion:

$$\begin{aligned} & \beta_{\frac{n}{2}-1}[v_i(\frac{n}{2}-1) + v_i(\frac{n}{2}+2)] = \beta_{\frac{n}{2}-1} v_i(\frac{n}{2}-1) + \beta_{\frac{n}{2}+1} v_i(\frac{n}{2}+2) \\ = \;& [(\lambda_i - a(\frac{n}{2}))v_i(\frac{n}{2}) - \beta_{\frac{n}{2}} v_i(\frac{n}{2}+1)] + [(\lambda_i - a(\frac{n}{2}+1))v_i(\frac{n}{2}+1) - \beta_{\frac{n}{2}} v_i(\frac{n}{2})] \\ \geq \;& [\lambda_i - a(\frac{n}{2}) - \beta_{\frac{n}{2}}][v_i(\frac{n}{2}) + v_i(\frac{n}{2}+1)] \geq \beta_{\frac{n}{2}}[v_i(\frac{n}{2}) + v_i(\frac{n}{2}+1)] \geq 0. \end{aligned}$$

We now use induction backward to prove (3.36). Assume

$$\beta_k[v_i(k) + v_i(n+1-k)] \geq \beta_{k+1}[v_i(k+1) + v_i(n-k)]$$

for some $k > j$, then by (3.1), (3.33) and (3.34)

$$\begin{aligned}
& \beta_{k-1}[v_i(k-1) + v_i(n+2-k)] = \beta_{k-1}v_i(k-1) + \beta_{n+1-k}v_i(n+2-k)] \\
= & [(\lambda_i - a(k))v_i(k) - \beta_k v_i(k+1)] + [(\lambda_i - a(n+1-k))v_i(n+1-k) - \beta_{n-k}v_i(n-k)] \\
= & (\lambda_i - a(k))v_i(k) + (\lambda_i - a(n+1-k))v_i(n+1-k) - \beta_k[v_i(k+1) + v_i(n-k)] \\
= & [\lambda_i - a(k)][v_i(k) + v_i(n+1-k)] - \beta_k[v_i(k) + v_i(n+1-k)] \\
= & [\lambda_i - a(k) - \beta_k][v_i(k) + v_i(n+1-k)] \geq \beta_{k+1}[v_i(k+1) + v_i(n-k)] \geq 0.
\end{aligned}$$

as desired. □

Let's apply Theorem 3.10 to the previous example $J_{10}((2,2,0,0,0,0,0,0,2.1,2))$. We have $j = 2$ and eigenvalues

$$\lambda_n = 3.2467 > \lambda_{n-1} = 3.1915 > 2.$$

Under the normalization (3.35), Theorem 3.10 says that

$$s_i(2) + s_i(9) > s_i(3) + s_i(8) > s_i(4) + s_i(7) > s_i(5) + s_i(6)$$

for i=n and n-1. The numerical values given above satisfy these inequalities.

Chapter 4

The Minimal Gap

In this chapter we settle our minimization problem; to find the minimal gap among the class of matrices

$$\mathcal{L}_\omega^n := \{J(\mathbf{a}) |\ \mathbf{a} \in [0, \omega]^n\}$$

when ω is large enough. Formally we seek

$$\min\{g(J(\mathbf{a}))|\ 0 \leq a(k) \leq \omega \text{ for } k = 1, 2, \ldots, n\},$$

$$\text{or} \quad \min\{g_i(J(\mathbf{a}))|\ \mathbf{a} \in [0, \omega]^n \text{ and } i = 1, 2, \ldots, n-1\}. \tag{4.1}$$

The answer to this problem is stated precisely in Theorem 4.8. Section 4.5 gives the outline of our proof.

4.1 Ericsson's Lower Bound

Consider the tridiagonal matrix T of the form

$$\text{tridiag}\begin{pmatrix} & \beta_1 & \cdots & \beta_{n-1} & \\ a(1) & \cdot & \cdots & \cdots & a(n) \\ & \beta_1 & \cdots & \beta_{n-1} & \end{pmatrix} \tag{4.2}$$

with all β_i's positive. Let the eigenvalues of T be labeled as $\lambda_1 < \lambda_2 < \ldots < \lambda_n$, and $d = \lambda_n - \lambda_1$ be the eigenvalue spread of T. Assume $\mathbf{s_i} = (s_i(1), s_i(2), \ldots, s_i(n))$ is the i-th normalized eigenvector of T.

Theorem 4.1 (Ericsson [4]) $g(T) \geq 2\beta_1\beta_2 \cdots \beta_{n-1}/d^{n-2}$ *where* $d = \lambda_n - \lambda_1$.

Proof. Let

$$\chi(\lambda) =: det[\lambda I - T] = \prod_{k=1}^{n}(\lambda - \lambda_k)$$

and $\chi'(\lambda)$ be the derivative of $\chi(\lambda)$ with respect to λ. Then

$$s_i(1)s_i(n)\chi'(\lambda_i) = \prod_{k=1}^{n-1}\beta_k, \qquad \text{for } i = 1, 2, \ldots, n. \tag{4.3}$$

by Corollary 1.9 (i). Since the arithmetic mean exceeds the geometric mean,

$$1 = ||s_i||_2^2 = \sum_{k=1}^{n} s_i(k)^2 \geq s_i(1)^2 + s_i(n)^2 \geq 2\,|s_i(1)s_i(n)|,$$

and (4.3) gives

$$\prod_{k=1}^{i-1}(\lambda_i - \lambda_k)\prod_{k=i+1}^{n}(\lambda_k - \lambda_i) = |\chi'(\lambda_i)| \geq 2\prod_{k=1}^{n-1}\beta_k. \tag{4.4}$$

Pull out the $\lambda_{i+1} - \lambda_i$ term and bound the others by d in the left hand side of (4.4), then

$$(\lambda_{i+1} - \lambda_i)\, d^{n-2} \geq 2\prod_{k=1}^{n-1}\beta_k,$$

$$\text{i.e.} \quad \lambda_{i+1} - \lambda_i \geq 2\,(\prod_{k=1}^{n-1}\beta_k)/d^{n-2}$$

for $i = 1, 2, \ldots, n-1$. Hence we have the desired inequality by (1.3). □

Although the eigenvalues of T can be surprisingly close to each other as in W_{21}, according to Theorem 4.1 they cannot be arbitrarily close when the entries $a(i)$'s and β_i's are bounded. We remark that Theorem 4.1 can also be derived by Theorem 1.2, but Sun's method is different from ours. In addition we need the following refinement.

Theorem 4.2 *Given* $1 \leq i \leq n-1$. *Let* $m = \min\{i, n-i\}$ *and* d *be the spread of* T, *then*

$$g_i(T) \geq 2^{2m-1}\beta_1\beta_2\cdots\beta_{n-1}/d^{n-2}.$$

Proof. Assume $i \leq \frac{n}{2}$, then

$$\begin{aligned}
&\prod_{j=1}^{i-1}(\lambda_i - \lambda_j)\prod_{k=i+1}^{n}(\lambda_k - \lambda_i)\\
= &\prod_{j=1}^{i-1}(\lambda_i - \lambda_j)\cdot(\lambda_{i+1} - \lambda_i)\prod_{k=i+2}^{n-i+1}(\lambda_k - \lambda_i)\cdot\prod_{k=n-i+2}^{n}(\lambda_k - \lambda_i)
\end{aligned}$$

$$
\begin{aligned}
&= \prod_{j=1}^{i-1}(\lambda_i-\lambda_j)(\lambda_{n-j+1}-\lambda_i)\cdot(\lambda_{i+1}-\lambda_i)\cdot\prod_{k=i+2}^{n-i+1}(\lambda_k-\lambda_i)\\
&\le \prod_{j=1}^{i-1}\Big(\frac{\lambda_i-\lambda_j+\lambda_{n-j+1}-\lambda_i}{2}\Big)^2\cdot(\lambda_{i+1}-\lambda_i)\,d^{n-2i}\\
&\le \Big(\frac{d}{2}\Big)^{2(i-1)}(\lambda_{i+1}-\lambda_i)\,d^{n-2i}=\frac{d^{n-2}}{2^{2i-2}}(\lambda_{i+1}-\lambda_i).
\end{aligned}
$$

Therefore

$$g_i \ge 2^{2i-1}\Big(\prod_{k=1}^{n-1}\beta_k\Big)/d^{n-2}$$

by (4.4). The argument for $i > \frac{n}{2}$ is similar. □

This refined theorem says that the middle eigenvalue separations have bigger lower bounds than the end ones. Thus the middle separations cannot be too close compared to the end ones.

Now we can get a lower bound for the gaps in our class $\mathcal{L}_\omega^n$. The spectrum of $J(\mathbf{a})$ is contained in

$$[a(1)-1,a(1)+1]\cup\bigcup_{k=2}^{n-1}[a(k)-2,a(k)+2]\cup[a(n)-1,a(n)+1]$$

by Gershgorin's Disk Theorem. Since $a(k)\in[0,\omega]$, all the eigenvalues are in the interval $[-2,\omega+2]$ and the spread

$$d\le\omega+4.$$

Therefore by Theorem 4.1

$$g(J)\ge\frac{2}{d^{n-2}}\ge\frac{2}{(\omega+4)^{n-2}}$$

for $J\in\mathcal{L}_\omega^n$. Moreover by Theorem 4.2

$$g_i(J)\ge\frac{8}{(\omega+4)^{n-2}} \tag{4.5}$$

for $n\ge4$, $i=2,3,\ldots,n-2$ and $J\in\mathcal{L}_\omega^n$.

Recall that

$$g_{n-1}(J(\mathbf{w}_1))<\frac{2}{\omega^{n-2}}$$

by Theorem 2.3 (iii). Hence the minimum in (4.1) must be smaller than $\frac{2}{\omega^{n-2}}$. Thus all the middle g_i's in (4.5) are too large to consider provided that

$$\frac{8}{(\omega+4)^{n-2}}\ge\frac{2}{\omega^{n-2}}\quad\Leftrightarrow\quad 4>\Big(1+\frac{4}{\omega}\Big)^{n-2}\quad\Leftrightarrow\quad\omega>\frac{4}{\sqrt[n-2]{4}-1}. \tag{4.6}$$

The right hand side of (4.6) seems mysterious. Consider $\delta = \frac{1}{n-2}$, then

$$4^{\delta} = e^{\delta \ln 4} = 1 + \delta \ln 4 + \frac{1}{2}(\delta \ln 4)^2 + \cdots > 1 + \delta \ln 4$$

and

$$\frac{4}{4^{\delta} - 1} < \frac{4}{\delta \ln 4} = \frac{2}{\ln 2}(n-2).$$

The constant $\frac{2}{\ln 2} = 2.885390082 < 2.8854$. Therefore (4.6) holds if

$$\omega > 2.8854(n-2). \tag{4.7}$$

By more detailed analysis of the spread this constant can be reduced, but some constraint like (4.7) is necessary because of the counterexample in Table 1.2.

We conclude that the minimum of (4.1) comes from g_1 or g_{n-1} if ω is large enough. This is certainly trivial when $n = 3$. Recall that

$$g_1(J(\mathbf{a})) = g_{n-1}(J(\mathbf{a}^*))$$

by Corollary 1.5 (iii), where

$$\mathbf{a}^* = \omega\mathbf{e} - \mathbf{a} = (\omega - a(1), \omega - a(2), \ldots, \omega - a(n))$$

is the dual of $\mathbf{a}$ with respect to ω. Note that $\mathbf{a}^* \in [0, \omega]^n$ if and only if $\mathbf{a} \in [0, \omega]^n$. Therefore under the condition of (4.7), (4.1) is equivalent to

$$\min \{ g_{n-1}(J(\mathbf{a})) | \ \mathbf{a} \in [0, \omega]^n \}. \tag{4.8}$$

After the reduction, it suffices to solve (4.8).

4.2 Refinement Sun's Theorem

In this section we also consider the tridiagonal matrices $T(\mathbf{a})$ of the form (4.2) with positive β_k's. Sun's Theorem 1.2 is refined below. These inequalities say that $\lambda_{i+1} - \lambda_i$ cannot be too small when $i \geq \frac{n}{2}$ and the trace of T is large, or when $i < \frac{n}{2}$ and the trace of T is small.

Theorem 4.3 *Let $\overline{\lambda}_n$ be an upper bound for λ_n and $\underline{\lambda}_1$ be a lower bound for λ_1. Define*

$$\acute{q} := \frac{1}{n-2}\left[\sum_{k=1}^{n-1} a(k) - (n-1)\underline{\lambda}_1\right], \qquad \grave{q} := \frac{1}{n-2}\left[(n-1)\overline{\lambda}_n - \sum_{k=1}^{n-1} a(k)\right],$$

$$\acute{r} := \frac{1}{n-2}\left[\sum_{k=2}^{n} a(k) - (n-1)\underline{\lambda}_1\right], \qquad \grave{r} := \frac{1}{n-2}\left[(n-1)\overline{\lambda}_n - \sum_{k=2}^{n} a(k)\right],$$

$$\acute{t} := \frac{1}{n-2}\left[\frac{a(1)+a(n)}{2} + \sum_{k=2}^{n-1} a(k) - (n-1)\underline{\lambda}_1\right],$$

$$\grave{t} := \frac{1}{n-2}\left[(n-1)\overline{\lambda}_n - \frac{a(1)+a(n)}{2} - \sum_{k=2}^{n-1} a(k)\right],$$

$$\bar{q} = \max\{\acute{q}, \grave{q}\}, \qquad \bar{r} = \max\{\acute{r}, \grave{r}\}, \qquad \bar{t} = \max\{\acute{t}, \grave{t}\}.$$

Then

i. $g_i(T(\mathbf{a})) \geq 2(\prod_{k=1}^{n-1} \beta_k)/(\acute{q}\acute{r})^{\frac{n}{2}-1}$, $\quad g_i(T(\mathbf{a})) \geq 2(\prod_{k=1}^{n-1} \beta_k)/\acute{t}^{n-2}$ *for* $i = 1, 2, \ldots, [\frac{n-1}{2}]$;

ii. $g_i(T(\mathbf{a})) \geq 2(\prod_{k=1}^{n-1} \beta_k)/(\grave{q}\grave{r})^{\frac{n}{2}-1}$, $\quad g_i(T(\mathbf{a})) \geq 2(\prod_{k=1}^{n-1} \beta_k)/\grave{t}^{n-2}$ *for* $i = [\frac{n+1}{2}], \ldots, n-1$;

iii. $g(T(\mathbf{a})) \geq 2(\prod_{k=1}^{n-1} \beta_k)/(\bar{q}\bar{r})^{\frac{n}{2}-1}$, *and* $g(T(\mathbf{a})) \geq 2(\prod_{k=1}^{n-1} \beta_k)/\bar{t}^{n-2}$.

Proof. According to Corollary 1.9 (iv)

$$\chi_{1,n-1}(\lambda_i)\chi_{2,n}(\lambda_i) = \prod_{k=1}^{n-1} \beta_k^2,$$

where $\chi_{j,k}(\lambda) := \det[\lambda I - T_{j,k}]$ and

$$T_{j,k}(\mathbf{a}) := \operatorname{tridiag}\begin{pmatrix} & \beta_j & \cdots & \beta_{k-1} & \\ a(j) & \cdot & \cdots & \cdot & a(k) \\ & \beta_j & \cdots & \beta_{k-1} & \end{pmatrix} \qquad \text{for } j \leq k,$$

Let $\{\theta_k\}_{k=1}^{n-1}$ and $\{\mu_k\}_{k=1}^{n-1}$ be the eigenvalues of $T_{1,n-1}$ and $T_{2,n}$ respectively, in increasing order. Thus

$$\prod_{k=1}^{n-1}(\lambda_i - \theta_k)(\lambda_i - \mu_k) = \prod_{k=1}^{n-1} \beta_k^2 \qquad \text{for } i = 1, 2, \ldots, n. \tag{4.9}$$

Replace i by $i+1$ in (4.9) and multiply it by (4.9), then

$$\prod_{k=1}^{n-1}(\lambda_i - \theta_k)(\lambda_{i+1} - \theta_k)(\lambda_i - \mu_k)(\lambda_{i+1} - \mu_k) = \prod_{k=1}^{n-1} \beta_k^4. \tag{4.10}$$

Recall that $\lambda_k < \theta_k < \lambda_{k+1}$ and $\lambda_k < \mu_k < \lambda_{k+1}$ for $k = 1, 2, \ldots, n-1$ by Cauchy's Interlacing Theorem [9, 10-1-2]. Since the arithmetic mean is no less than the geometric mean, we have

$$\left[\prod_{k=1}^{i-1}(\lambda_i - \theta_k) \prod_{k=i+1}^{n-1} (\theta_k - \lambda_i)\right]^{\frac{1}{n-2}}$$

$$
\begin{aligned}
&\leq \frac{1}{n-2}[\sum_{k=1}^{i-1}(\lambda_i-\theta_k)+\sum_{k=i+1}^{n-1}(\theta_k-\lambda_i)] \\
&= \frac{1}{n-2}[(2i-n)\lambda_i-\sum_{k=1}^{i-1}\theta_k+\sum_{k=i+1}^{n-1}\theta_k] \\
&= \begin{cases} \frac{1}{n-2}[(2i-n)\lambda_i-\theta_i-2\sum_{k=1}^{i-1}\theta_k+\sum_{k=1}^{n-1}\theta_k], & \text{if } i<\frac{n}{2} \\ \frac{1}{n-2}[(2i-n)\lambda_i+\theta_i+2\sum_{k=i+1}^{n-1}\theta_k-\sum_{k=1}^{n-1}\theta_k], & \text{if } i\geq\frac{n}{2} \end{cases} \\
&\leq \begin{cases} \frac{1}{n-2}[tr(T_{1,n-1})-(n-1)\lambda_1]\leq\acute{q}, & \text{if } i<\frac{n}{2} \\ \frac{1}{n-2}[(n-1)\lambda_n-tr(T_{1,n-1})]\leq\grave{q}, & \text{if } i\geq\frac{n}{2} \end{cases}
\end{aligned}
$$

since $\sum_{k=1}^{n-1}\theta_k = tr(T_{1,n-1}) = \sum_{k=1}^{n-1}a(k)$. Thus for $i<\frac{n}{2}$, (4.10) gives

$$
\begin{aligned}
\prod_{k=1}^{n}\beta_k^4 &= (\theta_i-\lambda_i)(\lambda_{i+1}-\theta_i)(\mu_i-\lambda_i)(\lambda_{i+1}-\mu_i)\cdot \\
&\quad \prod_{k=1}^{i-1}(\lambda_i-\theta_k)(\lambda_{i+1}-\theta_k)(\lambda_i-\mu_k)(\lambda_{i+1}-\mu_k)\cdot \\
&\quad \prod_{k=i}^{n-1}(\theta_k-\lambda_i)(\theta_k-\lambda_{i+1})(\mu_k-\lambda_i)(\mu_k-\lambda_{i+1}) \\
&\leq [\frac{\theta_i-\lambda_i+\lambda_{i+1}-\theta_i}{2}]^2[\frac{\mu_i-\lambda_i+\lambda_{i+1}-\mu_i}{2}]^2\acute{q}^{n-2}\acute{q}^{n-2}\acute{r}^{n-2}\acute{r}^{n-2} \\
&= (\frac{g_i}{2})^4\acute{q}^{2n-4}\acute{r}^{2n-4},
\end{aligned}
$$

i.e. $\qquad g_i \geq 2(\prod_{k=1}^{n-1}\beta_k)/(\acute{q}\acute{r})^{\frac{n}{2}-1} \qquad$ for $i=1,2,\ldots,[\frac{n-1}{2}]$.

It is exactly the same when $i\geq\frac{n}{2}$. Clearly gap

$$g(T)\geq 2(\prod_{k=1}^{n-1}\beta_k)/(\bar{q}\bar{r})^{\frac{n}{2}-1}.$$

Again use the inequality of arithmetic and geometric means

$$(\acute{q}\acute{r})^{\frac{1}{2}}\leq\frac{1}{2}(\acute{q}+\acute{r})=\acute{t},$$

and

$$(\grave{q}\grave{r})^{\frac{1}{2}}\leq\frac{1}{2}(\grave{q}+\grave{r})=\grave{t}.$$

The other half follows in the same way. $\square$

Theorem 4.3 is slightly better than Theorem 1.2 since

$$p_2 = \frac{1}{n-2}(n\overline{\lambda}_n - \sum_{k=1}^{n} a_k) \geq \dot{t} \quad \text{and} \quad p_3 = \frac{1}{n-2}(\sum_{k=1}^{n} a_k - n\underline{\lambda}_1) \geq \acute{t}$$

by

$$\lambda_1 \leq \min_{k=1,2,\ldots,n}\{a(k)\} \qquad \text{and} \qquad \lambda_n \geq \max_{k=1,2,\ldots,n}\{a(k)\}.$$

For Wilkinson's matrix W_{2m+1}, $\overline{\lambda}_n = m+1$ and

$$\dot{q} = \dot{r} = \dot{t} = \frac{m^2+2m}{2m-1}.$$

Hence by Theorem 4.3

$$g_{n-1}(W_{2m+1}) \geq 2(\frac{2m-1}{m^2+2m})^{2m-1},$$

which yields 1.24×10^{-15} for W_{21} as in Table 1.1.

Now we can apply Theorem 4.3 to the class of matrices $\mathcal{L}^n_\omega$.

Corollary 4.4 *Suppose $J \in \mathcal{L}^n_\omega$ with $tr(J) \geq 3\omega$. If $\omega \geq 2n$, then $g_i(J) \geq \frac{2}{\omega^{n-2}}$ for $i = [\frac{n+1}{2}], \ldots, n-1$.*

Proof. For $J \in \mathcal{L}^n_\omega$, $\lambda_n \leq \omega + 2$. So we choose $\overline{\lambda}_n = \omega + 2$. Recall that

$$\overline{\lambda}_n \geq \lambda_n \geq \max_{k=1,2,\ldots,n}\{a(k)\} \geq \max\{a(1), a(n)\} \geq \frac{a(1)+a(n)}{2},$$

then

$$\begin{aligned}
\dot{t} &= \frac{1}{n-2}\left[(n-1)\overline{\lambda}_n - \frac{a(1)+a(n)}{2} - \sum_{k=2}^{n-1} a(k)\right] \\
&\leq \frac{1}{n-2}\left[n\overline{\lambda}_n - \sum_{k=1}^{n} a(k)\right] \quad \leq \frac{1}{n-2}\left[n(\omega+2) - 3\omega\right] \\
&\leq \frac{1}{n-2}\left[(n-3)\omega + 2n\right] \quad \leq \frac{1}{n-2}\left[(n-3)\omega + \omega\right] = \omega.
\end{aligned}$$

Thus by Theorem 4.3 (ii)

$$g_i \geq 2/\dot{t}^{n-2} \geq 2/\omega^{n-2}.$$

for $i = [\frac{n+1}{2}], \ldots, n-1$. □

As a consequence of Corollary 4.4 and Theorem 2.3 (iii),

$$g_{n-1}(J) \geq \frac{2}{\omega^{n-2}} > g_{n-1}(J(\mathbf{w_1})),$$

if $tr(J) \geq 3\omega$ and

$$\omega \geq 2n. \tag{4.11}$$

Hence under the condition (4.11), the minimizer of (4.8) must have trace less than 3ω.

4.3 Unsymmetric Diagonal

From Section 3.2, $\nabla g_{n-1}(J(\mathbf{a}))$ has only three types of sign pattern

I. $(-,-,\ldots,-,+0,+,\ldots,+,+0)$;

II. $(+0,+,\ldots,+,+0,-,-,\ldots,-)$;

III. $(-,\ldots,-,+0,+,\ldots,+,+0,-,\ldots,-)$.

Here "+0" means the entry can be positive or zero.

Since ∇g_{n-1} never vanishes, the global minimum point $\mathbf{a}$ of (4.8) must be a boundary point of $[0,\omega]^n$ which satisfies the Kuhn-Tucker condition. Since all the possible sign patterns of gradients are known, the corresponding minimizers can be only

I. $(\omega,\omega,\ldots,\omega,*,0,\ldots,0,*)$;

II. $(*,0,\ldots,0,*,\omega,\omega,\ldots,\omega)$;

III. $(\omega,\ldots,\omega,*,0,\ldots,0,*,\omega,\ldots,\omega)$.

Here " * " means the entry can be anything in $[0,\omega]$.

To be a minimizer, it is impossible to have too many ω's in the diagonal. Courtesy of the result in the end of last section, at most two ω's are allowed in the diagonal if $\omega \geq 2n$. The possible minimizers are thus reduced to five cases

i. $\mathbf{a} = (x,0,\ldots,0,y,\omega,\omega)$ with $\nabla g_{n-1} = (+0,+,\ldots,+,+0,-,-)$;

ii. $\mathbf{a} = (x,0,0,\ldots,0,y,\omega)$ with $\nabla g_{n-1} = (+0,+,+,\ldots,+,+0,-)$;

iii. $\mathbf{a} = (\omega,x,0,\ldots,0,y,\omega)$ with $\nabla g_{n-1} = (-,+0,+,\ldots,+,+0,-)$;

iv. $\mathbf{a} = (\omega,\omega,y,0,\ldots,0,x)$ with $\nabla g_{n-1} = (-,-,+0,+,\ldots,+,+0)$;

v. $\mathbf{a} = (\omega,y,0,\ldots,0,0,x)$ with $\nabla g_{n-1} = (-,+0,+,\ldots,+,+,+0)$;

We want to show that none of the unbalanced diagonal $\mathbf{a}$ can be the minimizer. The following lemma is crucial.

Lemma 4.5 *Assume* $s_n(1)s_{n-1}(1) > 0$, $\lambda_{n-1} > 2$,

$$a(k) \leq a(n+1-k) \qquad \textit{for } k = 1,2,\ldots,j,$$

with at least one strict inequality, and

$$a(k) = 0 \qquad \textit{for } k = j+1, j+2, \ldots, n-j,$$

for some integer $j \leq [\frac{n+1}{2}]$, *Then*

$$\frac{s_{n-1}(j)}{s_n(j)} > -\frac{s_{n-1}(n+1-j)}{s_n(n+1-j)}.$$

Proof. By assumption, we have at least one strict inequality in (3.28). Without loss of generality, choose both $s_n(1)$ and $s_{n-1}(1)$ positive, then

$$s_n(k) < s_n(n+1-k) \qquad \text{for } k = 1, 2, \ldots, [\frac{n}{2}] \tag{4.12}$$

by Theorem 3.8, and

$$s_{n-1}(\frac{n+1}{2}) > 0 \text{ for odd } n, \qquad \text{and } s_{n-1}(\frac{n}{2}) + s_{n-1}(\frac{n}{2}+1) > 0 \text{ for even } n$$

by Theorem 3.9. Hence according to Theorem 3.10

$$s_{n-1}(j) + s_{n-1}(n+1-j) \geq 0. \tag{4.13}$$

Notice that $s_{n-1}(j)$ must be positive, otherwise

$$s_{n-1}(1) > 0, \quad s_{n-1}(j) \leq 0 \quad \text{and} \quad s_{n-1}(n+1-j) \geq 0,$$

by (4.13), which violates that $\mathbf{s}_{n-1}$ has only one sign change. Therefore, using (4.12) and (4.13),

$$\frac{s_{n-1}(j)}{s_n(j)} > \frac{s_{n-1}(j)}{s_n(n+1-j)} \geq -\frac{s_{n-1}(n+1-j)}{s_n(n+1-j)}.$$

□

In all the cases above, $\lambda_n \geq \max_{k=1,2,\ldots,n}\{a(k)\} \geq \omega$. Suppose $\omega > 3$ and $n \geq 3$. If $\lambda_{n-1} \leq \omega - 1$, then

$$\lambda_n - \lambda_{n-1} \geq 1 > \frac{2}{\omega^{n-2}} > g_{n-1}(J(\mathbf{w}_1)),$$

which is clearly not competitive. Hence in the sequel we assume $\lambda_{n-1} > \omega - 1 > 2$ Also we take $s_n(1), s_{n-1}(1) > 0$.

Obviously case (i) satisfies Lemma 4.5. Assume the $(n-2)$-th entry of ∇g_{n-1} is zero, i.e.

$$\frac{s_{n-1}(n-2)}{s_n(n-2)} = -1.$$

Then by Lemma 4.5

$$1 > \frac{s_{n-1}(3)}{s_n(3)} > -\frac{s_{n-1}(n-2)}{s_n(n-2)} = 1,$$

which is impossible. Therefore the $(n-2)$-th entry of ∇g_{n-1} must be positive and y must vanish. Case (i) thus reduces to

$$\mathbf{a} = (x, 0, \ldots, 0, 0, \omega, \omega) \quad \text{with} \quad \nabla g_{n-1} = (+0, +, \ldots, +, +, -, -).$$

Notice that

$$\frac{s_{n-1}(n-1)}{s_n(n-1)} < -1.$$

By Lemma 4.5 again, we have

$$1 > \frac{s_{n-1}(2)}{s_n(2)} > -\frac{s_{n-1}(n-1)}{s_n(n-1)} > 1,$$

a contradiction. We conclude that there is no diagonal $\mathbf{a}$ in case (i) such that $\nabla g_{n-1}(J(\mathbf{a}))$ satisfies the desired sign pattern.

To exclude $\mathbf{w}_1$ from case (ii), either $x < \omega$ or $y > 0$. Assume the $(n-1)$-th entry of ∇g_{n-1} is zero, i.e.

$$\frac{s_{n-1}(n-1)}{s_n(n-1)} = -1.$$

Then by Lemma 4.5

$$1 > \frac{s_{n-1}(2)}{s_n(2)} > -\frac{s_{n-1}(n-1)}{s_n(n-1)} = 1,$$

which is impossible. Thus the $(n-2)$-th entry of ∇g_{n-1} must be positive and y must vanish. Case (ii) then reduces to

$$\mathbf{a} = (x, 0, \ldots, 0, \omega) \quad \text{with} \quad \nabla g_{n-1} = (+0, +, \ldots, +, -).$$

Notice that

$$\frac{s_{n-1}(n)}{s_n(n)} < -1.$$

Again Lemma 4.5 forces a contradiction

$$1 \geq \frac{s_{n-1}(1)}{s_n(1)} > -\frac{s_{n-1}(n)}{s_n(n)} > 1,$$

In summary there is no $\mathbf{a}$ in case (ii), except $\mathbf{w}_1$, with the desired sign pattern of ∇g_{n-1}.

Similarly we assume $x < y$ in case (iii). Then $y > 0$ and the $(n-2)$-th entry of ∇g_{n-1} must vanish. In other words

$$\frac{s_{n-1}(n)}{s_n(n)} = -1.$$

By Lemma 4.5 again we reaches a contradiction

$$1 \geq \frac{s_{n-1}(1)}{s_n(1)} > -\frac{s_{n-1}(n)}{s_n(n)} = 1,$$

The counter part $x > y$ can be eliminated similarly.

Notice that (iv) and (v) are symmetric to (i) and (ii), hence they can be dealt in the same fashion and the only possibility is $\mathbf{w_1}$.

Therefore only the symmetric diagonal $\mathbf{a} = (\omega, x, 0, \ldots, 0, x, \omega)$ in case (iii) survived our test. Since we have ruled out the situation when trace $\geq 3\omega$ by (4.11), we only need to consider $x \leq \frac{\omega}{2}$. This will be discussed in the next section.

4.4 Isolated Minimum

In this section we consider (4.8) with $\mathbf{a}$ near $\mathbf{w_1}$. Assume $n \geq 4$, $0 \leq x \leq \frac{\omega}{2}$ and diagonal vector

$$\mathbf{u}(x) = (\omega, x, 0, \ldots, 0, x, \omega).$$

We want to show $\nabla g_{n-1}(J(\mathbf{u}))$ has sign pattern

$$(-, +, +, \ldots, +, +, -) \tag{4.14}$$

if ω is sufficiently large. Hence $J(\mathbf{w_1})$ satisfies the Kuhn-Tucker condition on the boundary of $[0, \omega]^n$. Restricted to the class of admissible matrices $\mathcal{L}_\omega^n$, g_{n-1} attains a relative minimum at $J(\mathbf{w_1})$. Moreover $J(\mathbf{u}(x))$ can not be the minimizer for any $x \in (0, \frac{\omega}{2}]$.

Lemma 4.6 *Assume $n \geq 4$ and $0 \leq x \leq \frac{\omega}{2}$, then*

i. $\quad \omega < \lambda_{n-1}(J(\mathbf{u}(x))) < \lambda_n(J(\mathbf{u}(x))) < \omega + \frac{4}{\omega}$,

ii. $\quad g_{n-1}(J(\mathbf{u}(x))) < \frac{4}{\omega}$.

Proof. The Weyl's Monotonicity Theorem [5, Corollary 4.3.3] says that all the eigenvalues of a symmetric matrix increase if a positive semidefinite matrix is added to it. Therefore, by Theorem 2.3 (ii),

$$\lambda_{n-1}(J(\mathbf{u}(x))) > \lambda_{n-1}(J(\mathbf{w_1})) > \omega + \frac{1}{\omega - 2\omega^{1-n}} - \frac{1}{\omega^{n-2}} > \omega.$$

Consider

$$\mathbf{u}'(x) = (\omega - x, 0, \ldots, 0, \omega - x) \quad \text{and} \quad \mathbf{e} = (1, 1, \ldots, 1).$$

Then by Theorem 2.3 (i)

$$\lambda_n(J(\mathbf{u}'(x))) < \omega - x + \frac{1}{\omega - x} + \frac{1}{(\omega - x)^{n-2}} < \omega - x + \frac{2}{\omega - x} < \omega - x + \frac{4}{\omega}.$$

By Monotonicity Theorem and Theorem 1.4 (i)

$$\lambda_n(J(\mathbf{w_1})) < \lambda_n(J(\mathbf{u}'(x) + x\mathbf{e})) = \lambda_n(J(\mathbf{u}'(x))) + x < \omega + \frac{4}{\omega}.$$

Obviously (ii) follows from (i). □

Theorem 4.7 *Assume $n \geq 4$ and $\omega > \sqrt{9n-14} + 2$. Then*

i. $\mathbf{w_1}$ locally minimizes $g_{n-1}(J(\mathbf{a}))$ over all $\mathbf{a} \in [0,\omega]^n$;

ii. for all $x \in (0, \frac{\omega}{2}]$, $(\omega, x, \ldots, x, \omega)$ is not the minimum point of $g_{n-1}(J(\mathbf{a}))$.

Proof. Since $J(\mathbf{u})$ is centrosymmetric, $\mathbf{s_i}$ is either symmetric or skew symmetric by Corollary 1.10 (i). Hence $\nabla g_{n-1}(J(\mathbf{u}))$ is symmetric and it suffices to prove that the first half of

$$\nabla g_{n-1}(J(\mathbf{u})) = (s_n(1)^2 - s_{n-1}(1)^2, s_n(2)^2 - s_{n-1}(2)^2, \ldots, s_n(n)^2 - s_{n-1}(n)^2). \tag{4.15}$$

has the desired sign pattern (4.14). Recall that

$$s_i(1)^2 = \frac{1}{\prod\limits_{\substack{k=1\\k\neq i}}^{n} |\lambda_k - \lambda_i|} \quad \text{and} \quad s_i(2)^2 = \frac{(\lambda_i - \omega)^2}{\prod\limits_{\substack{k=1\\k\neq i}}^{n} |\lambda_k - \lambda_i|}$$

for $i = 1, 2, \ldots, n$ by Corollary 1.10 (iii).

Since $\lambda_n > \lambda_{n-1} > \lambda_k$ for $k = 1, 2, \ldots, n-2$,

$$s_n(1)^2 = \frac{1}{\prod\limits_{k=1}^{n-1} |\lambda_n - \lambda_k|} < \frac{1}{\prod\limits_{\substack{k=1\\k\neq n-1}}^{n} |\lambda_{n-1} - \lambda_k|} = s_{n-1}(1)^2.$$

Hence the first component of (4.15) is negative.

For the second entries of (4.15), we need $s_n(2)^2 > s_{n-1}(2)^2$, so

$$\frac{(\lambda_n - \omega)^2}{\prod\limits_{k=1}^{n-1} |\lambda_n - \lambda_k|} > \frac{(\lambda_{n-1} - \omega)^2}{\prod\limits_{\substack{k=1\\k\neq n-1}}^{n} |\lambda_{n-1} - \lambda_k|},$$

$$\text{so} \quad (\frac{\lambda_n - \omega}{\lambda_{n-1} - \omega})^2 > \prod_{k=1}^{n-2} \frac{\lambda_n - \lambda_k}{\lambda_{n-1} - \lambda_k},$$

$$\text{so} \quad (1 + \frac{g_{n-1}}{\lambda_{n-1} - \omega})^2 > \prod_{k=1}^{n-2} (1 + \frac{g_{n-1}}{\lambda_{n-1} - \lambda_k}). \tag{4.16}$$

By Lemma 4.6 (i)

$$\lambda_{n-1} - w < \lambda_n - \omega < \frac{4}{\omega},$$

so the left hand side of (4.16)

$$(1 + \frac{g_{n-1}}{\lambda_{n-1} - \omega})^2 \; > \; (1 + \frac{g_{n-1}\omega}{4})^2 \; = \; 1 + \frac{\omega}{2} g_{n-1} + \frac{\omega^2}{16} g_{n-1}^2. \tag{4.17}$$

Gershgorin's Disk Theorem gives the location of λ_i, which is contained in

$$[-2, 2] \bigcup [x - 2, x + 2] \bigcup [\omega - 1, \omega + 1].$$

Since $x \leq \frac{\omega}{2}$, the interval $[\omega - 1, \omega + 1]$ is well separated from the others if $\omega > 6$. In this case

$$\lambda_1 < \cdots < \lambda_{n-2} \leq x + 2 \leq \frac{\omega}{2} + 2$$

and by Lemma 4.6 (i)

$$\lambda_{n-1} - \lambda_k > \omega - (\frac{\omega}{2} + 2) = \frac{\omega}{2} - 2$$

for $k = 1, 2, \ldots, n-2$. The right hand side of (4.16)

$$\begin{aligned} \prod_{k=1}^{n-2} (1 + \frac{g_{n-1}}{\lambda_{n-1} - \lambda_k}) \; &< \; \prod_{k=1}^{n-2} (1 + \frac{g_{n-1}}{\omega/2 - 2}) \quad = (1 + \frac{2g_{n-1}}{\omega - 4})^{n-2} \\ &< \; (\exp \frac{2g_{n-1}}{\omega - 4})^{n-2} \quad = \exp[\frac{2(n-2)}{\omega - 4} g_{n-1}] \\ &= \; 1 + \frac{2(n-2)}{\omega - 4} g_{n-1} + \frac{e^{\eta}}{2} [\frac{2(n-2)}{\omega - 4}]^2 g_{n-1}^2. \end{aligned} \tag{4.18}$$

The last equality uses Taylor series expansion with the remainder term where $\eta \in (0, \frac{2(n-2)}{\omega-4} g_{n-1})$.

To have inequality (4.16), it suffices to compare the quadratic polynomials of g_{n-1} in (4.17) and (4.18). Assume

$$\frac{n-2}{\omega(\omega - 4)} < \frac{1}{9}. \tag{4.19}$$

The coefficients of g_{n-1} in (4.17) and (4.18) satisfy

$$\frac{2(n-2)}{\omega - 4} < \frac{2\omega}{9} < \frac{\omega}{2}.$$

Since

$$\eta < \frac{2g_{n-1}(n-2)}{\omega - 4} < \frac{8(n-2)}{\omega(\omega-4)} < \frac{8}{9}$$

by Lemma 4.6 (ii) and (4.10), the coefficients of g_{n-1}^2 in (4.17) and (4.18) obey

$$\frac{e^\eta}{2}[\frac{2(n-2)}{\omega-4}]^2 < \frac{e^{8/9}}{2}(\frac{2\omega}{9})^2 = \frac{2e^{8/9}}{81}\omega^2 < 0.061\omega^2 < \frac{\omega^2}{16}.$$

We conclude that (4.16), or equivalently $s_n(2)^2 - s_{n-1}(2)^2 > 0$, holds under (4.19). Rewrite (4.19)

$$\begin{aligned} \omega^2 - 4\omega > 9(n-2) \quad &\Longleftrightarrow \quad (\omega-2)^2 > 9n - 14 \\ &\Longleftrightarrow \quad \omega > \sqrt{9n-14} + 2. \end{aligned} \tag{4.20}$$

Notice that when $n \geq 4$

$$\omega > \sqrt{9 \cdot 4 - 14} + 2 = \sqrt{22} + 2 \approx 6.69 > 6.$$

Recall that the ratio of $s_{n-1}(k)$ and $s_n(k)$ satisfies

$$\left|\frac{s_{n-1}(1)}{s_n(1)}\right| > \left|\frac{s_{n-1}(2)}{s_n(2)}\right| > \cdots \left|\frac{s_{n-1}([\frac{n+1}{2}])}{s_n([\frac{n+1}{2}])}\right|.$$

by Theorem 3.2. Thus

$$\begin{aligned} (4.20) \quad &\Longrightarrow \quad s_n(2)^2 > s_{n-1}(2)^2 \\ &\Longrightarrow \quad 1 > \left|\frac{s_{n-1}(2)}{s_n(2)}\right| > \left|\frac{s_{n-1}(3)}{s_n(3)}\right| > \cdots \left|\frac{s_{n-1}([\frac{n+1}{2}])}{s_n([\frac{n+1}{2}])}\right| \\ &\Longrightarrow \quad s_n(k)^2 > s_{n-1}(k)^2 \qquad \text{for } 2, 3, \ldots, [\frac{n+1}{2}]. \end{aligned}$$

Hence (4.15) has the desired sign pattern by symmetry. □

4.5 Global Minimum

We have solved, as promised, the minimization problem

$$\min\{g(J(\mathbf{a}))|\ \mathbf{a} \in [0, \omega]^n\} \tag{4.21}$$

for ω large enough: $g_{n-1}(J(\mathbf{w_1}))$ is the minimum. We now outline the whole argument.

One key idea is to use our candidate $g_{n-1}(J(\mathbf{w_1}))$ as an eliminator. Since

$$g_{n-1}(J(\mathbf{w_1})) < \frac{2}{\omega^{n-2}}$$

by Theorem 2.3 (iii), the minimum in (4.21) must be smaller than $\frac{2}{\omega^{n-2}}$. Hence we can throw away all the $J(\mathbf{a})$ with eigenvalue separations not less than $\frac{2}{\omega^{n-2}}$.

For the class of matrices $\mathcal{L}_\omega^n$ of interest, their spectra are contained in $[-2, \omega+2]$ by Gershgorin's Disk Theorem. Thus the spread d of each $J \in \mathcal{L}_\omega^n$ is less than $w + 4$. By Theorem 4.2

$$g_i(J) \geq \frac{8}{(\omega+4)^{n-2}} \geq \frac{2}{\omega^{n-2}}$$

for $i = 2, 3, \ldots, n-2$ if

$$n \geq 4 \quad \text{and} \quad \omega > 2.8854(n-2). \tag{4.22}$$

Hence under the assumption (4.22), the minimum of (4.21) comes from g_1 or g_{n-1}. The constant 2.8854 is not the best possible, however, some condition on ω/n is necessary.

Duality, introduced in Section 1.3, shows that there cannot be a unique minimizer since

$$g_1(J(\mathbf{a})) = g_{n-1}(J(\mathbf{a}^*))$$

by Corollary 1.5 (iii), where

$$\mathbf{a}^* = \omega\mathbf{e} - \mathbf{a} = (\omega - a(1), \omega - a(2), \ldots, \omega - a(n))$$

is the dual of $\mathbf{a}$ with respect to ω. Note that $\mathbf{a}^* \in [0,\omega]^n$ if and only if $\mathbf{a} \in [0,\omega]^n$. Therefore under the condition of (4.22), (4.21) is reduced to

$$\min \{\, g_{n-1}(J(\mathbf{a}))|\ \mathbf{a} \in [0,\omega]^n \}. \tag{4.23}$$

Now we have a smooth functional to minimize.

Another key idea is to use the trace to eliminate rivals to $J(\mathbf{w_1})$. As a consequence of Corollary 4.4, for $J \in \mathcal{L}_\omega^n$ with $tr(J) \geq 3\omega$,

$$g_{n-1}(J) \geq \frac{2}{\omega^{n-2}} > g_{n-1}(J(\mathbf{w_1})),$$

provided that

$$\omega \geq 2n. \tag{4.24}$$

Again some condition on ration ω/n is necessary and (4.24) probably can be improved. Anyhow the minimizer of (4.23) must have trace less than 3ω if we assume (4.24).

The global minimum of (4.23) must be a relative minimum subject to the constraint and obeys the Kuhn-Tucker condition: the diagonal $\mathbf{a}$ needs to match the sign pattern of

$\nabla g_{n-1}(J(\mathbf{a}))$. Since all the possible sign patterns of gradients are known from Section 3.2, we can obtain all the possible minimizers.

Under (4.24), the possible minimizers finally reduced to five cases

i. $\mathbf{a} = (x, 0, \ldots, 0, y, \omega, \omega)$ with $\nabla g_{n-1} = (+0, +, \ldots, +, +0, -, -)$;

ii. $\mathbf{a} = (x, 0, 0, \ldots, 0, y, \omega)$ with $\nabla g_{n-1} = (+0, +, +, \ldots, +, +0, -)$;

iii. $\mathbf{a} = (\omega, x, 0, \ldots, 0, y, \omega)$ with $\nabla g_{n-1} = (-, +0, +, \ldots, +, +0, -)$;

iv. $\mathbf{a} = (\omega, \omega, y, 0, \ldots, 0, x)$ with $\nabla g_{n-1} = (-, -, +0, +, \ldots, +, +0)$;

v. $\mathbf{a} = (\omega, y, 0, \ldots, 0, 0, x)$ with $\nabla g_{n-1} = (-, +0, +, \ldots, +, +, +0)$.

All the cases with unsymmmetric diagonal $\mathbf{a}$ are impossible. This is courtesy of Lemma 4.5. Therefore only the symmetric diagonal $\mathbf{u}(x) = (\omega, x, 0, \ldots, 0, x, \omega)$ in case (iii) survives. By the requirement of trace $\geq 3\omega$, we only need to consider $x \leq \frac{\omega}{2}$.

In Theorem 4.7 we show $\nabla g_{n-1}(J(\mathbf{u}))$ has sign pattern $(-, +, +, \ldots, +, +, -)$ if

$$n \geq 4 \quad \text{and} \quad \omega > \sqrt{9n - 14} + 2. \tag{4.25}$$

Hence among all $\mathbf{u}(x)$'s, only $\mathbf{w_1}$ satisfies the Kuhn-Tucker condition on the boundary of $[0, \omega]^n$, and is the unique minimizer for (4.8).

Under the assumptions of $\omega \geq 3$, (4.24) and (4.25), $J(\mathbf{w_1})$ uniquely minimizes (4.23). Notice that

$$\begin{aligned} 2n > \sqrt{9n - 14} + 2 \quad &\Longleftrightarrow \quad (2n-2)^2 > 9n - 4 \\ \Longleftrightarrow \quad 4n^2 - 17n + 18 > 0 \quad &\Longleftrightarrow \quad (4n-9)(n-2) > 0 \end{aligned}$$

is true if $n \geq 4$. Since $\omega \geq 2n \geq 8 > 3$, only the conditions $n \geq 4$ and (4.24) are needed.

For (4.21), we have two minimizers $J(\mathbf{w_1})$ and $J(\mathbf{w_1}^*)$ if (4.22) and (4.24) hold. Compare the right hand sides of (4.22) and (4.24)

$$2.8854(n-2) \geq 2n \Longleftrightarrow .8854n \geq 5.7708 \Longleftrightarrow n \geq 6.518.$$

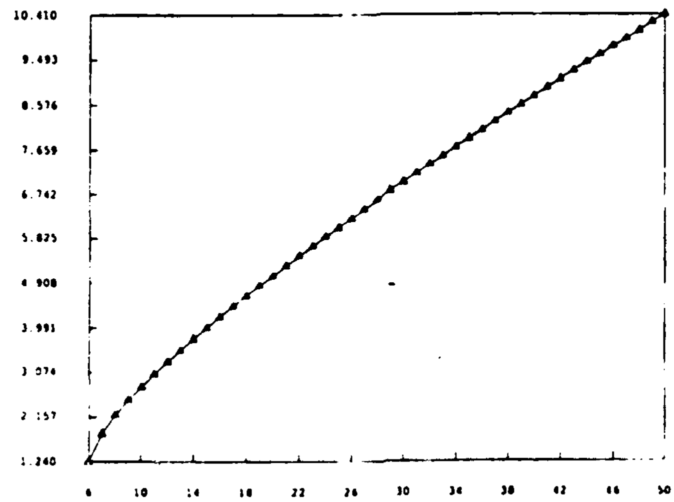

Figure 4.1: Graph of $\varpi(n)$ in $[6, 50]$.

Theorem 4.8 *i. Assume $n \geq 4$ and $\omega \geq 2n$, then $\mathbf{w_1}$ uniquely minimizes $g_{n-1}(J(\mathbf{a}))$ over all $\mathbf{a} \in [0, \omega]^n$.*

ii. Assume $n \geq 4$ and $\omega \geq 2n$, then $\mathbf{w_1}^*$ uniquely minimizes $g_1(J(\mathbf{a}))$ over all $\mathbf{a} \in [0, \omega]^n$.

iii. Assume $n \geq 7$ and $\omega \geq 2.8854(n-2)$, then $\mathbf{w_1}$ and $\mathbf{w_1}^*$ are the only minimizers of $g(J(\mathbf{a}))$ over all $\mathbf{a} \in [0, \omega]^n$. For $n = 4, 5, 6$, we need $\omega \geq 2n$.

This result shows that $J(\mathbf{w_1})$ and $J(\mathbf{w_1}^*)$ are the extremal matrices of the class $\mathcal{L}_\omega^n$ for ω large enough. More precisely, Theorem 4.8 requires

$$\omega \geq 2n \qquad \text{or} \qquad \omega \geq 2.8854(n-2). \tag{4.26}$$

However as mentioned, neither inequality is sharp. For each n, there is a value $\omega = \varpi(n)$ such that

$$g_{n-1}(J(\mathbf{w_1})) = g_{n-1}(J(\mathbf{w_2})),$$

for which $J(\mathbf{w_1})$ and $J(\mathbf{w_2})$ are both minimizers. Theorem 4.8 holds for $\omega \geq \varpi(n)$, and this inequality is then the best possible.

We have not been able to determine the functional form of $\varpi(n)$, but by using Mathematica with up to 70 decimal digit precision, we computed $\varpi(n)$ for $n = 6, 7, \ldots, 50$ to two digits of accuracy. The graph is displayed in Figure 4.1 and appears to grow a little less than linearly. In fact,

$$0.21n + 0.87 > \varpi(n) > 0.21n - 0.1 \qquad \text{for} \quad 6 \leq n \leq 50.$$

So the conditions (4.26) are of the right order of magnitute.

From Figure 4.1, we expect

$$\varpi(n) \longrightarrow \infty \qquad \text{as} \quad n \longrightarrow \infty.$$

When the size of diagonal spread ω is fixed, Theorem 4.8 holds for only a finite number of n's.

Bibliography

[1] M. S. Ashbaugh and R. D. Benguria. Some eigenvalue inequalities for a class of jacobi matrices. submitted to Linear Algebra and Its Applications.

[2] M. S. Ashbaugh and R. D. Benguria. Optimal lower bound for the gap between the first two eigenvalues of one-dimensional schrodinger operators with symmetric single-well potentials. *Proc. Amer. Math. Soc.*, 105: 419–424, 1989.

[3] A. Cantoni and P. Butler. Eigenvalues and eigenvectors of symmetric centrosymmetric matrices. *Linear Algebra and Its Applications*, 13: 275–288, 1976.

[4] T. Ericsson. Private communication, 1985.

[5] R. A. Horn and C. R. Johnson. *Matrix Analysis.* Cambridge University Press, New York, 1985.

[6] W. Kirsch and B. Simon. Universal lower bounds on eigenvalue splittings for one dimensional schrodinger operators. *Comm. Math. Phys.*, 97: 453–460, 1985.

[7] W. Kirsch and B. Simon. Comparison theorems for the gap of schrodinger operators. *J. Funct. Anal.*, 75: 396–410, 1987.

[8] C. C. Paige. *The computation of eigenvalues and eigenvectors of very large sparse matrices.* PhD thesis, University of London, 1971.

[9] B. N. Parlett. *The Symmetric Eigenvalue Problem.* Prentice-Hall, Englewood, N.J., 1980.

[10] B. N. Parlett. Given eigenvector recurrence revisited. Invited talk at the Proceedings of the 1st International SIAM meeting, ICIAM, Minisymposium in honor of J. H. Wilkinson, Paris, July 1987.

[11] I. M. Singer, B. Wang, S.-T. Yau, and S. S.-T. Yau. An estimate of the gap of the first two eigenvalues in the schrodinger operator. *Ann. Scuola Norm. Sup. Pisa Ser. 4*, 12: 319–333, 1985.

[12] J.-C. Sun. On the minimum eigenvalue separation for matrices. *Mathematica Numerica Sinica*, 7(3), 1985.

[13] R. C. Thompson and P. McEnteggert. Principal submatrices II, the upper and lower quadratic inequalities. *Linear Algebra and Its Applications*, 1: 211–243, 1968.

[14] B.-Y. Wang. The bounds of minimum eigenvalue separation of some matrices. *Mathematica Numerica Sinica*, 5(2): 176–186, 1983.

[15] J. H. Wilkinson. *The Algebraic Eigenvalue Problem.* Oxford University, New York, 1965.

[16] Q. Yu and J.-Q. Zhong. Lower bounds on the gap between the first and second eigenvalues of schrodinger operator. *Trans. Amer. Math. Soc.*, 294: 341–349, 1986.

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